



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 10:50 am BST

PDB ID : 8AKN / pdb_00008akn
EMDB ID : EMD-15488
Title : Cryo-EM structure of the proline-rich antimicrobial peptide drosocin bound to the terminating ribosome
Authors : Koller, T.O.; Morici, M.; Wilson, D.N.
Deposited on : 2022-07-30
Resolution : 2.30 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:

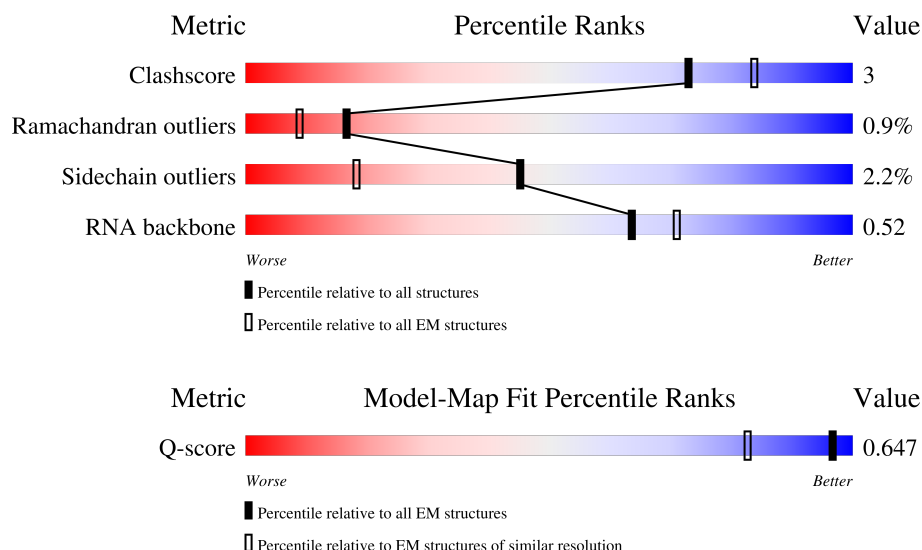
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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	
2	1	46	
3	2	65	

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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	19	
7	B	1534	
8	C	241	
9	D	233	
10	E	206	
11	F	167	
12	G	135	
13	H	179	
14	I	130	
15	J	130	
16	K	103	
17	L	129	
18	M	124	
19	N	118	
20	O	101	
21	P	89	
22	Q	82	
23	R	84	
24	S	75	
25	T	92	
26	U	87	
27	V	71	
28	W	360	

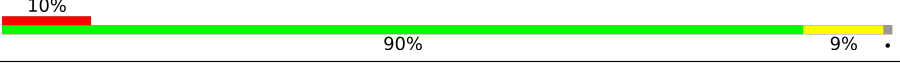
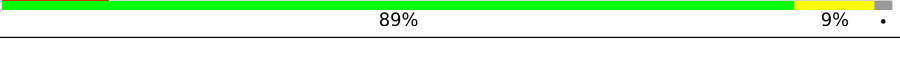
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Mol	Chain	Length	Quality of chain
29	X	76	
30	Y	9	
31	Z	76	
32	a	2903	
33	b	120	
34	c	273	
35	d	209	
36	e	201	
37	f	179	
38	g	177	
39	h	149	
40	i	142	
41	j	123	
42	k	144	
43	l	136	
44	m	127	
45	n	117	
46	o	115	
47	p	118	
48	q	103	
49	r	110	
50	s	100	
51	t	104	
52	u	94	
53	v	85	

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Mol	Chain	Length	Quality of chain
54	w	78	
55	x	63	
56	y	59	
57	z	57	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 146513 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 50S ribosomal protein L33.

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 50S ribosomal protein L34.

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 50S ribosomal protein L35.

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 50S ribosomal protein L36.

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 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a protein called Drosocin1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	A	19	Total	C	N	O	0	0
			155	98	34	23		

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	1519	Total	C	N	O	P	0	0
			32608	14548	5986	10555	1519		

- Molecule 8 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 9 is a protein called 30S ribosomal protein S3.

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

- Molecule 10 is a protein called 30S ribosomal protein S4.

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

- Molecule 11 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 12 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 14 is a protein called 30S ribosomal protein S8.

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

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

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

- Molecule 17 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 18 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 19 is a protein called 30S ribosomal protein S13.

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

- Molecule 20 is a protein called 30S ribosomal protein S14.

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

- Molecule 21 is a protein called 30S ribosomal protein S15.

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

- Molecule 22 is a protein called 30S ribosomal protein S16.

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

- Molecule 23 is a protein called 30S ribosomal protein S17.

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

- Molecule 24 is a protein called 30S ribosomal protein S18.

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

- Molecule 25 is a protein called 30S ribosomal protein S19.

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

- Molecule 26 is a protein called 30S ribosomal protein S20.

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

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 28 is a protein called Peptide chain release factor RF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	354	Total	C	N	O	S	0	0
			2792	1708	518	553	13		

- Molecule 29 is a RNA chain called Phenylalanine-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	9	Total	C	N	O	P	0	0
			188	85	31	63	9		

- Molecule 31 is a RNA chain called Isoleucine-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	76	Total	C	N	O	P	0	0
			1616	722	287	532	75		

- Molecule 32 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	2753	Total	C	N	O	P	0	0
			59128	26382	10897	19096	2753		

- Molecule 33 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 34 is a protein called 50S ribosomal protein L2.

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

- Molecule 35 is a protein called 50S ribosomal protein L3.

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

- Molecule 36 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 37 is a protein called 50S ribosomal protein L5.

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

- Molecule 38 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 39 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 40 is a protein called 50S ribosomal protein L13.

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

- Molecule 41 is a protein called 50S ribosomal protein L14.

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

- Molecule 42 is a protein called 50S ribosomal protein L15.

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

- Molecule 43 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 44 is a protein called 50S ribosomal protein L17.

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

- Molecule 45 is a protein called 50S ribosomal protein L18.

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

- Molecule 46 is a protein called 50S ribosomal protein L19.

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

- Molecule 47 is a protein called 50S ribosomal protein L20.

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

- Molecule 48 is a protein called 50S ribosomal protein L21.

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

- Molecule 49 is a protein called 50S ribosomal protein L22.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 51 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 52 is a protein called 50S ribosomal protein L25.

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

- Molecule 53 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 54 is a protein called 50S ribosomal protein L28.

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

- Molecule 55 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 56 is a protein called 50S ribosomal protein L30.

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

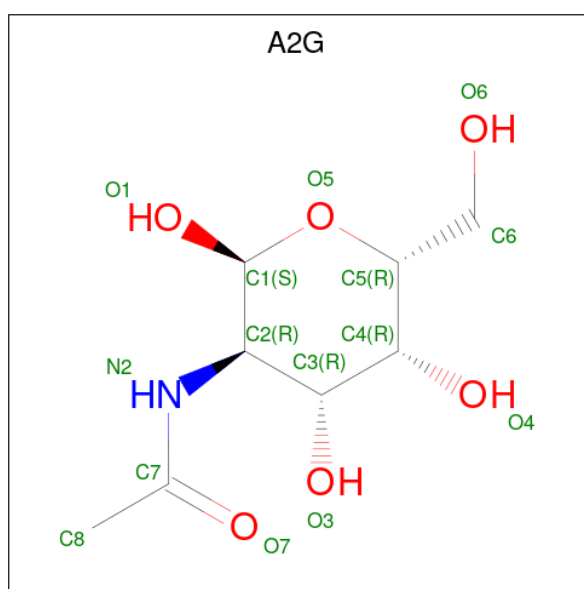
- Molecule 57 is a protein called 50S ribosomal protein L32.

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

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	3	1	Total	Zn	0
			1	1	
58	4	1	Total	Zn	0
			1	1	

- Molecule 59 is 2-acetamido-2-deoxy- α -D-galactopyranose (CCD ID: A2G) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

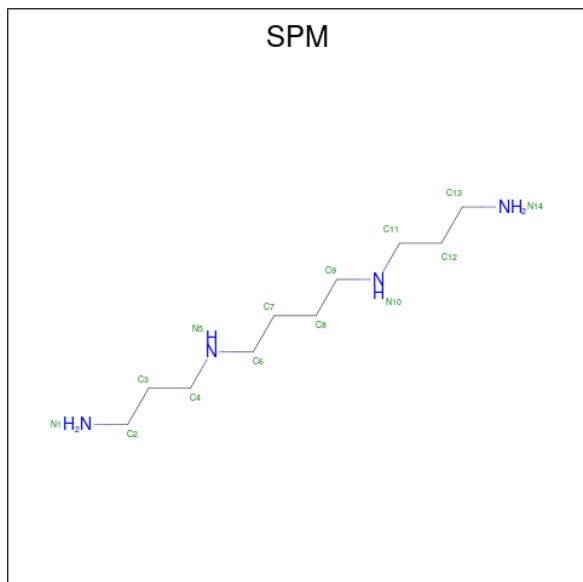


Mol	Chain	Residues	Atoms				AltConf
59	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	B	89	Total	Mg	0
			89	89	
60	a	208	Total	Mg	0
			208	208	
60	b	5	Total	Mg	0
			5	5	
60	c	1	Total	Mg	0
			1	1	
60	d	1	Total	Mg	0
			1	1	
60	z	1	Total	Mg	0
			1	1	

- Molecule 61 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
61	a	1	Total	C	N	0
			14	10	4	

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
62	0	1	Total	O	0
			1	1	
62	1	2	Total	O	0
			2	2	
62	2	12	Total	O	0
			12	12	

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Mol	Chain	Residues	Atoms		AltConf
62	3	3	Total 3	O 3	0
62	A	16	Total 16	O 16	0
62	B	189	Total 189	O 189	0
62	D	2	Total 2	O 2	0
62	E	1	Total 1	O 1	0
62	F	2	Total 2	O 2	0
62	M	2	Total 2	O 2	0
62	N	1	Total 1	O 1	0
62	R	1	Total 1	O 1	0
62	W	18	Total 18	O 18	0
62	X	1	Total 1	O 1	0
62	Y	6	Total 6	O 6	0
62	a	1331	Total 1331	O 1331	0
62	b	10	Total 10	O 10	0
62	c	41	Total 41	O 41	0
62	d	20	Total 20	O 20	0
62	e	15	Total 15	O 15	0
62	h	1	Total 1	O 1	0
62	i	2	Total 2	O 2	0
62	j	5	Total 5	O 5	0
62	k	16	Total 16	O 16	0

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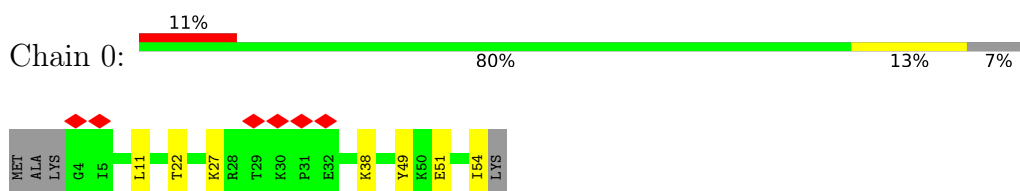
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Mol	Chain	Residues	Atoms		AltConf
62	l	8	Total 8	O 8	0
62	m	8	Total 8	O 8	0
62	n	1	Total 1	O 1	0
62	o	5	Total 5	O 5	0
62	p	8	Total 8	O 8	0
62	q	3	Total 3	O 3	0
62	r	7	Total 7	O 7	0
62	s	1	Total 1	O 1	0
62	t	1	Total 1	O 1	0
62	u	1	Total 1	O 1	0
62	v	3	Total 3	O 3	0
62	w	3	Total 3	O 3	0
62	z	7	Total 7	O 7	0

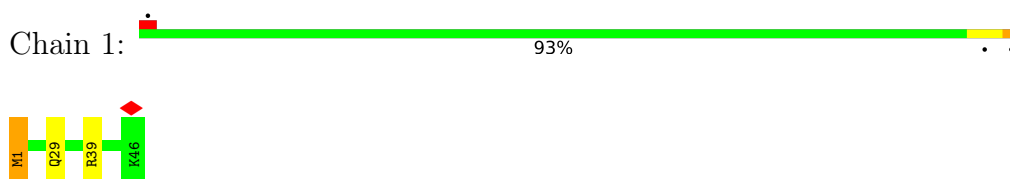
3 Residue-property plots [i](#)

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

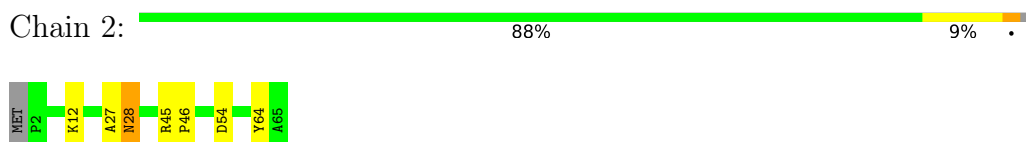
- Molecule 1: 50S ribosomal protein L33



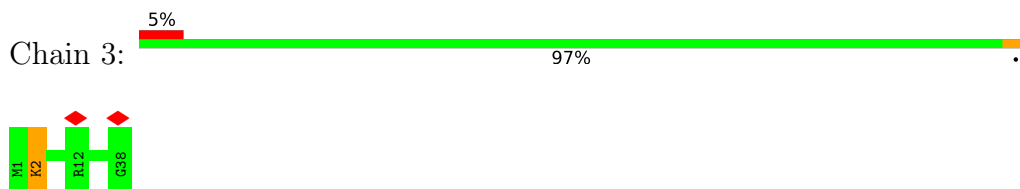
- Molecule 2: 50S ribosomal protein L34



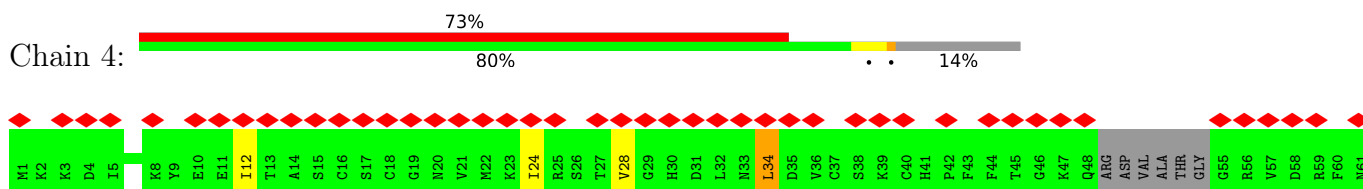
- Molecule 3: 50S ribosomal protein L35

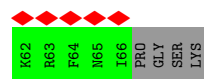


- Molecule 4: 50S ribosomal protein L36



- Molecule 5: 50S ribosomal protein L31





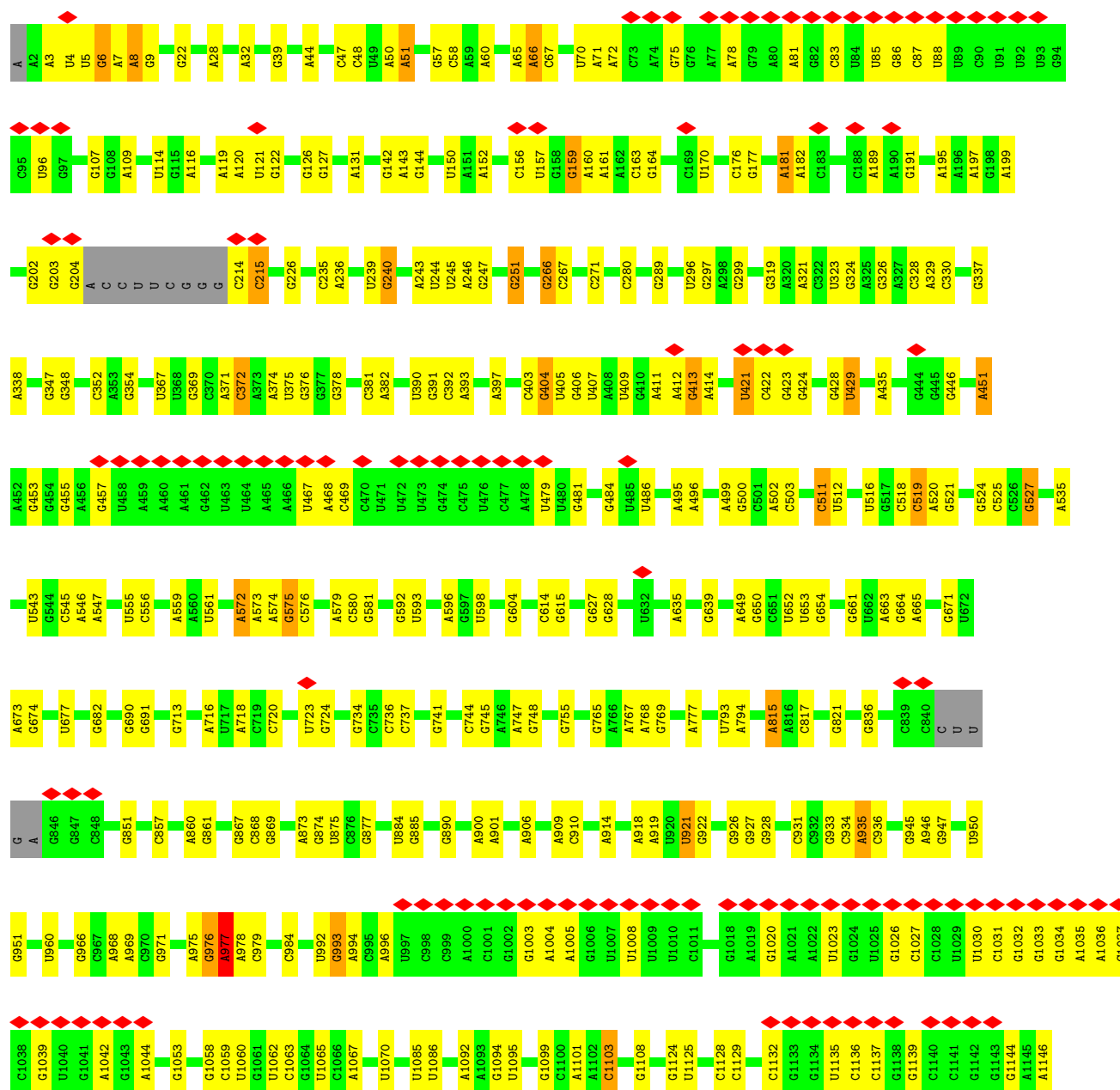
• Molecule 6: Drosocin1

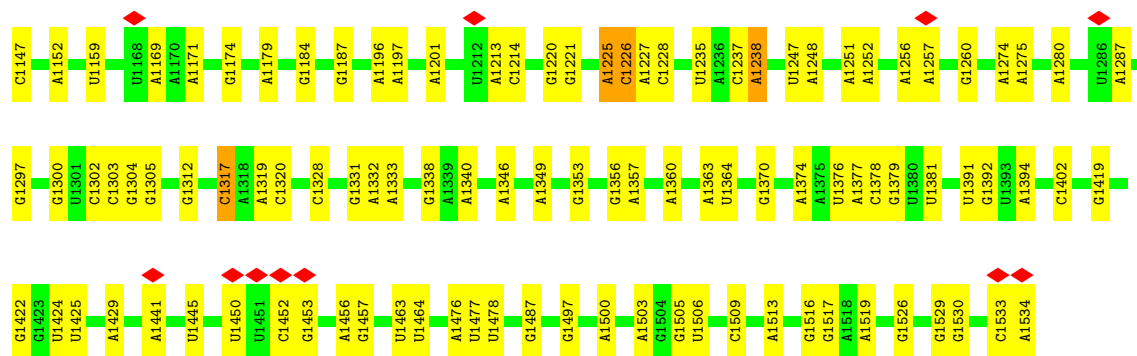
Chain A: 79% 16% 5%



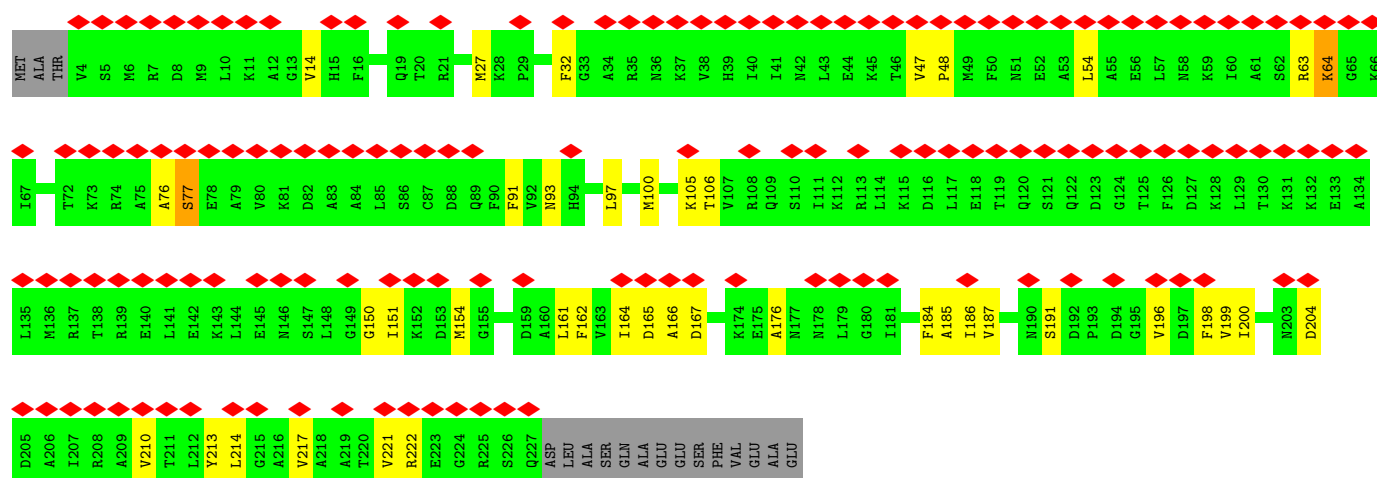
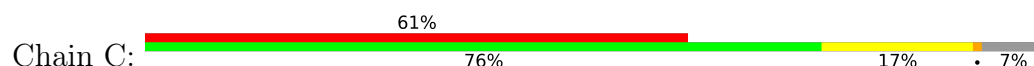
• Molecule 7: 16S ribosomal RNA

Chain B: 9% 71% 26% ..

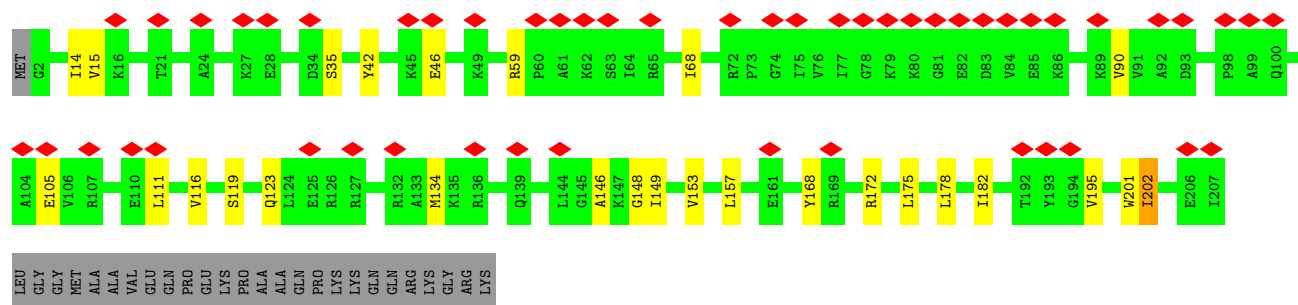
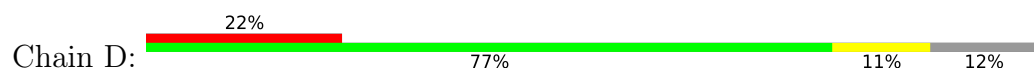




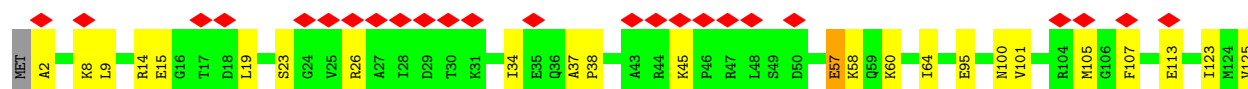
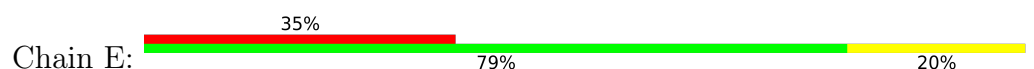
• Molecule 8: 30S ribosomal protein S2

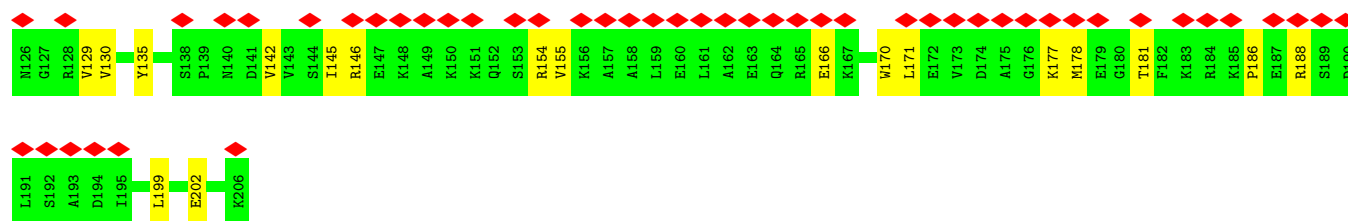


• Molecule 9: 30S ribosomal protein S3



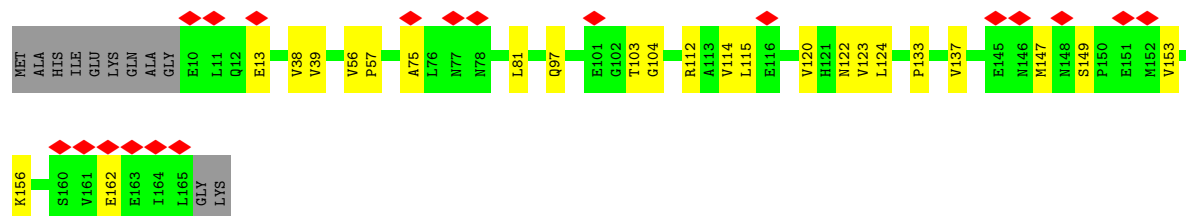
• Molecule 10: 30S ribosomal protein S4





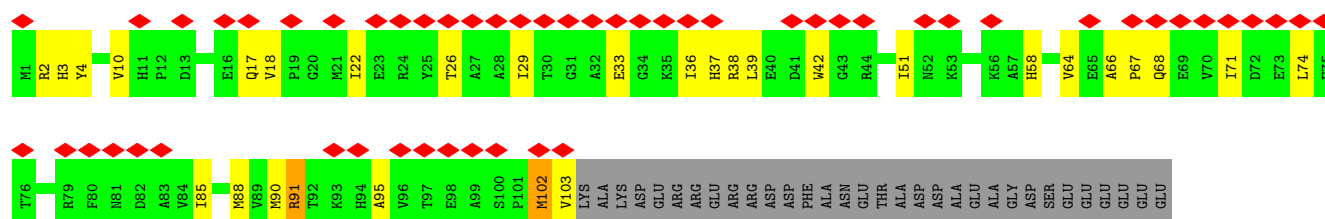
- Molecule 11: 30S ribosomal protein S5

Chain F:



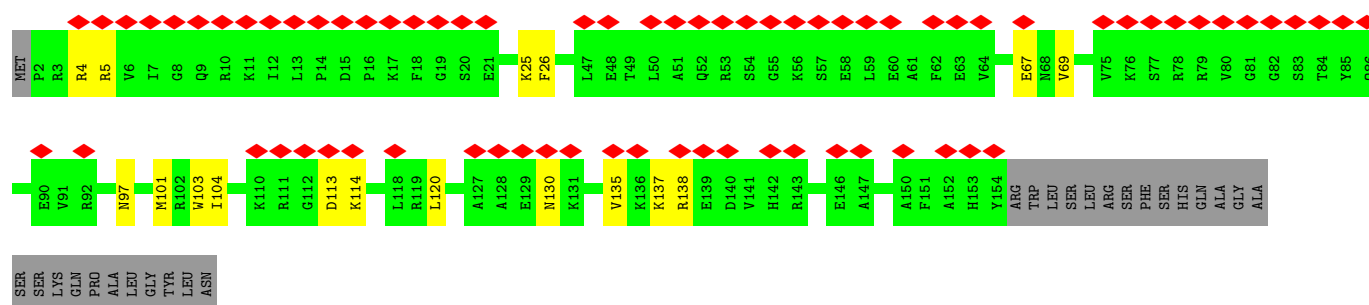
- Molecule 12: 30S ribosomal protein S6, fully modified isoform

Chain G:



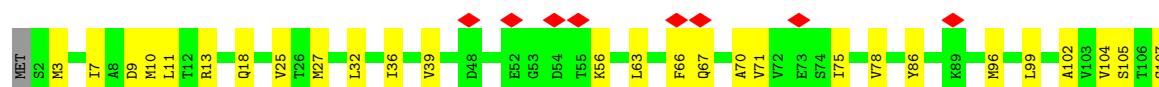
- Molecule 13: 30S ribosomal protein S7

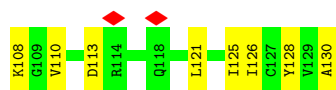
Chain H:



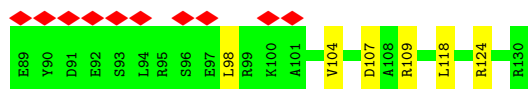
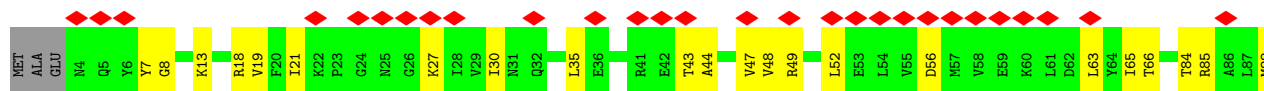
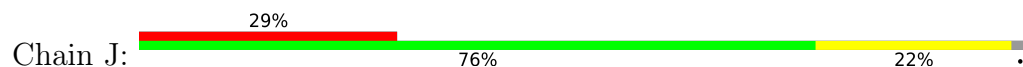
- Molecule 14: 30S ribosomal protein S8

Chain I:

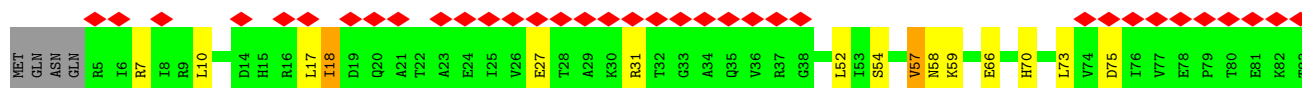
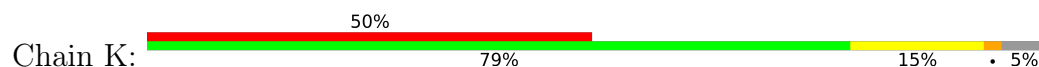




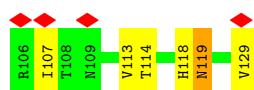
- Molecule 15: 30S ribosomal protein S9



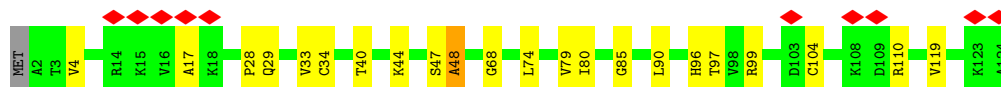
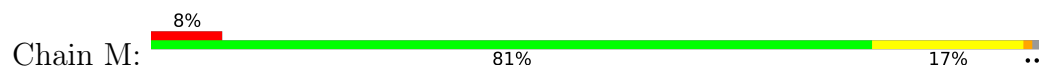
- Molecule 16: 30S ribosomal protein S10



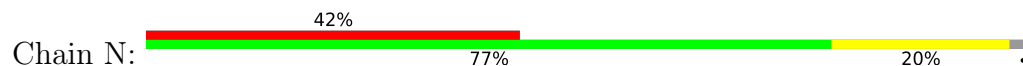
- Molecule 17: 30S ribosomal protein S11

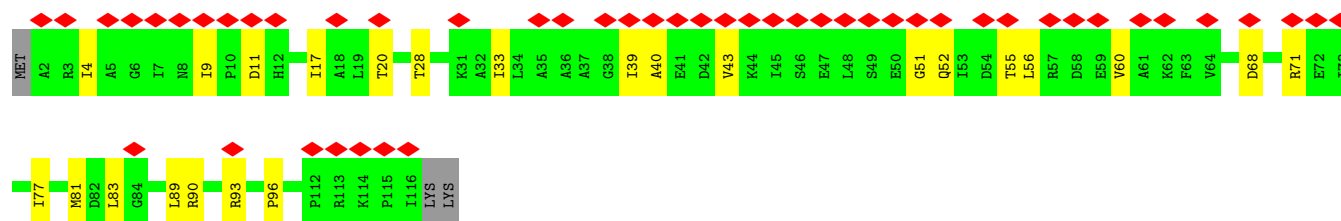


- Molecule 18: 30S ribosomal protein S12

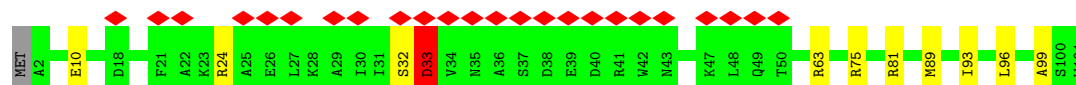
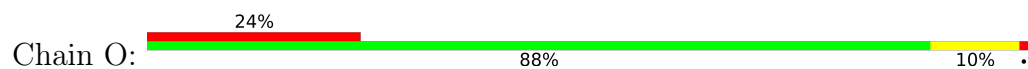


- Molecule 19: 30S ribosomal protein S13

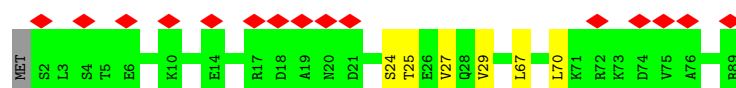
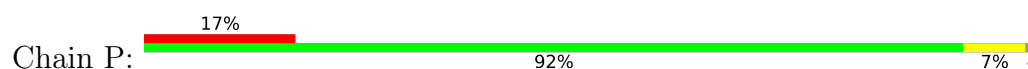




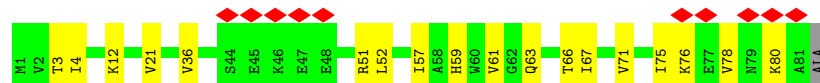
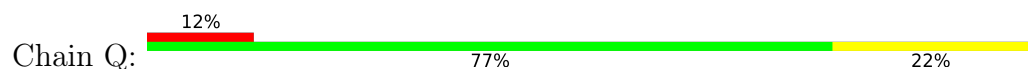
- Molecule 20: 30S ribosomal protein S14



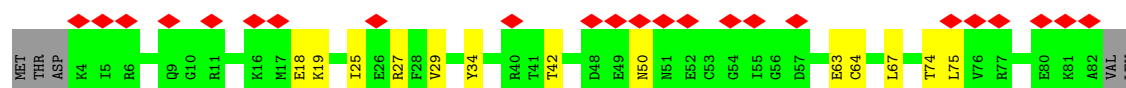
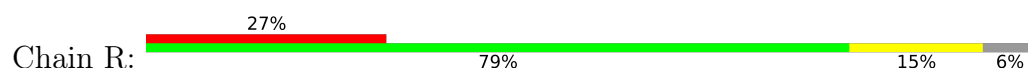
- Molecule 21: 30S ribosomal protein S15



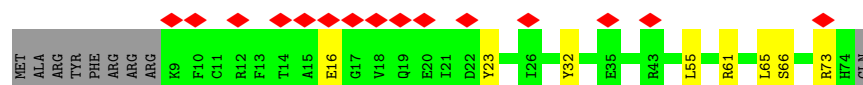
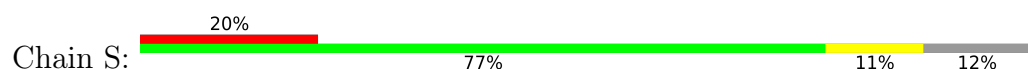
- Molecule 22: 30S ribosomal protein S16



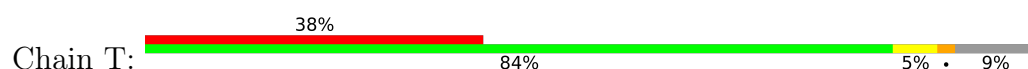
- Molecule 23: 30S ribosomal protein S17

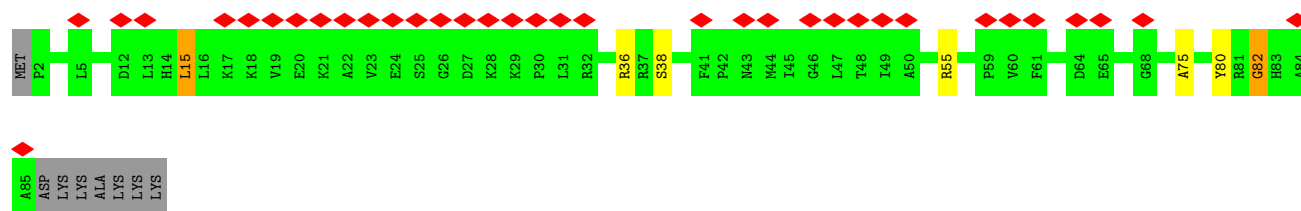


- Molecule 24: 30S ribosomal protein S18

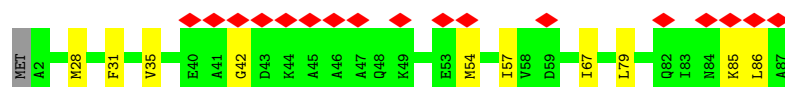
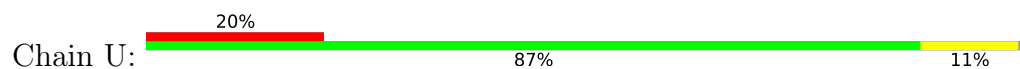


- Molecule 25: 30S ribosomal protein S19

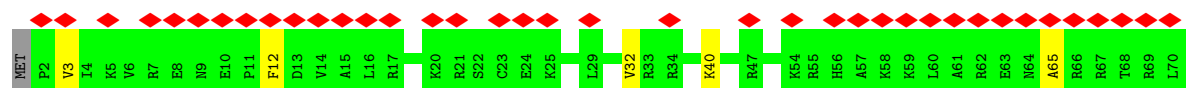
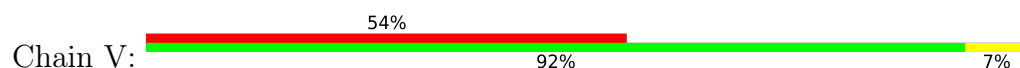




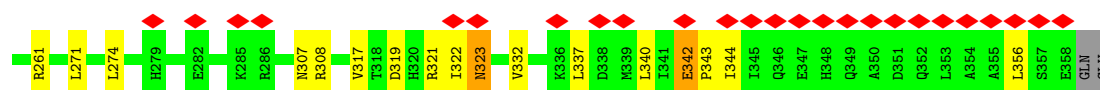
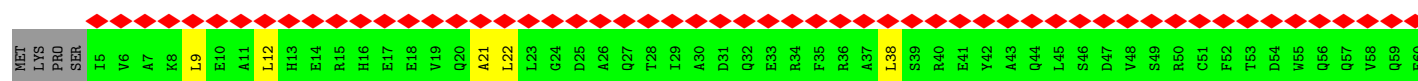
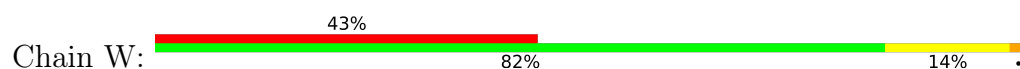
- Molecule 26: 30S ribosomal protein S20



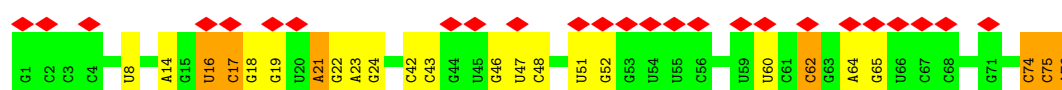
- Molecule 27: 30S ribosomal protein S21



- Molecule 28: Peptide chain release factor RF1



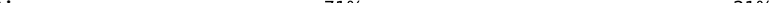
- Molecule 29: Phenylalanine-tRNA

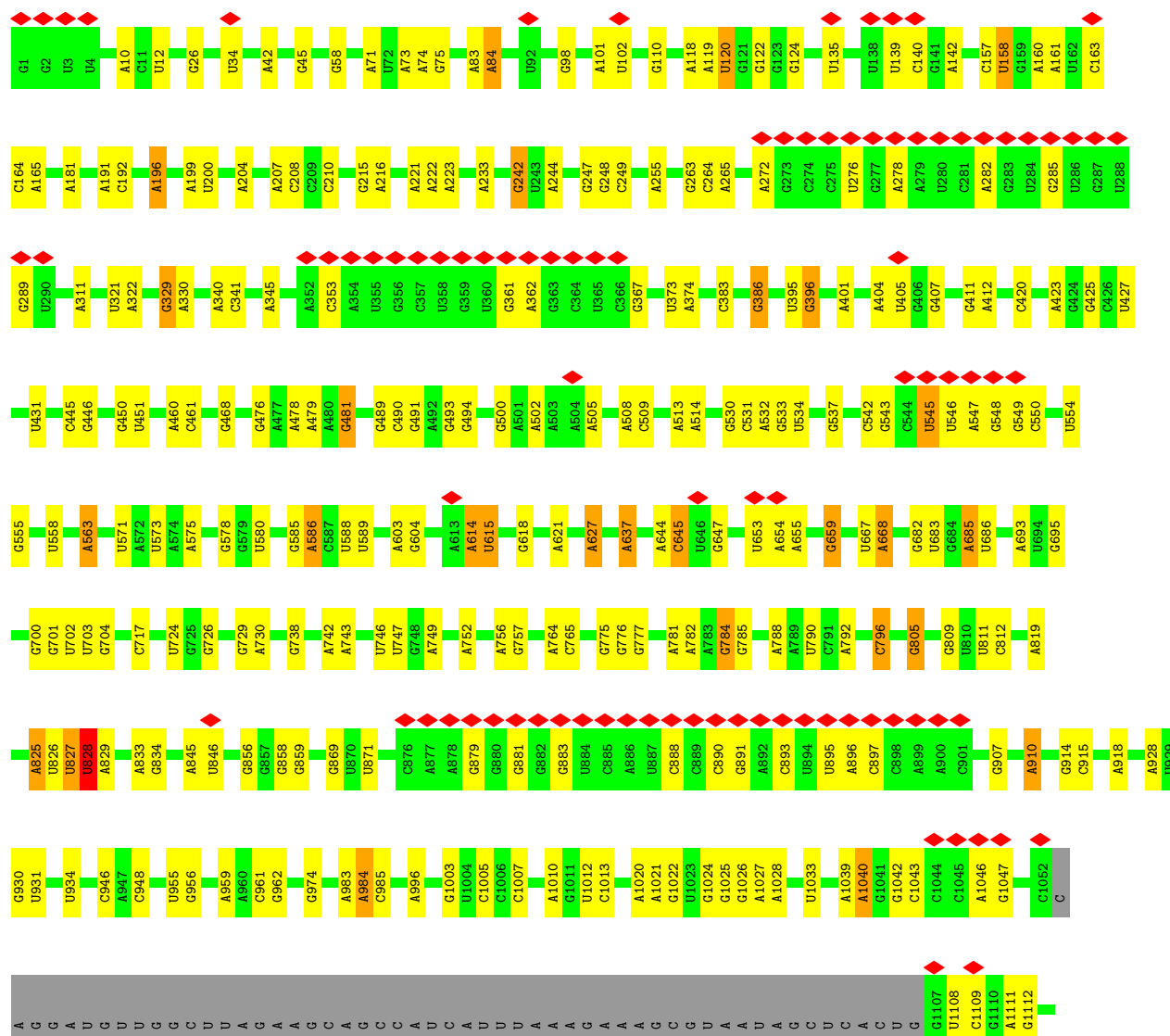


- Molecule 30: mRNA

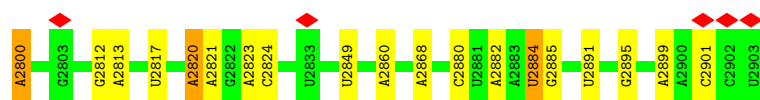
There are no outlier residues recorded for this chain.

Chain Z: 96% 45% 53%

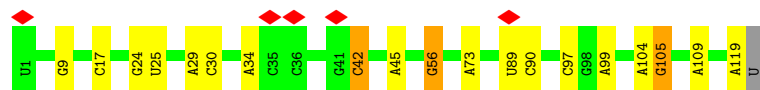
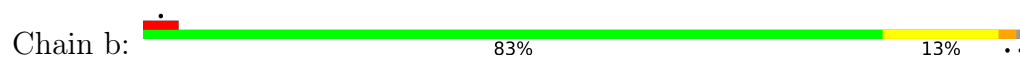
Chain a:  6% 71% 21% 5%



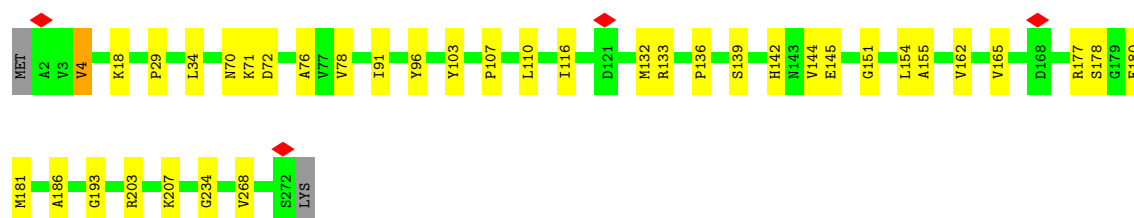
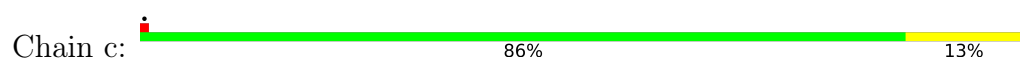




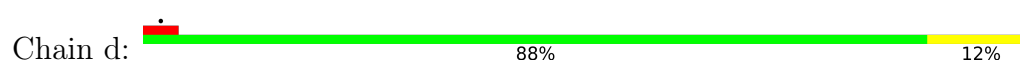
• Molecule 33: 5S ribosomal RNA



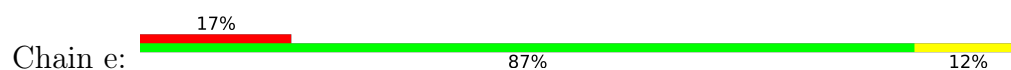
• Molecule 34: 50S ribosomal protein L2



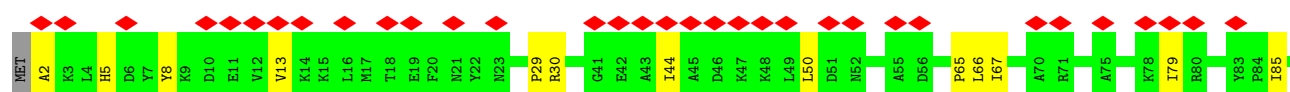
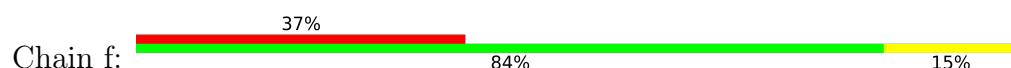
• Molecule 35: 50S ribosomal protein L3

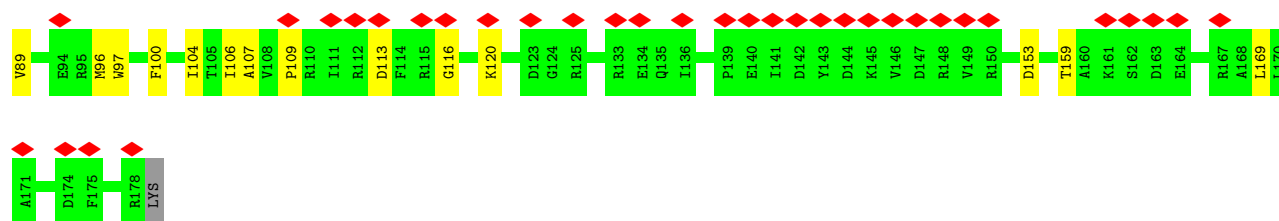


• Molecule 36: 50S ribosomal protein L4

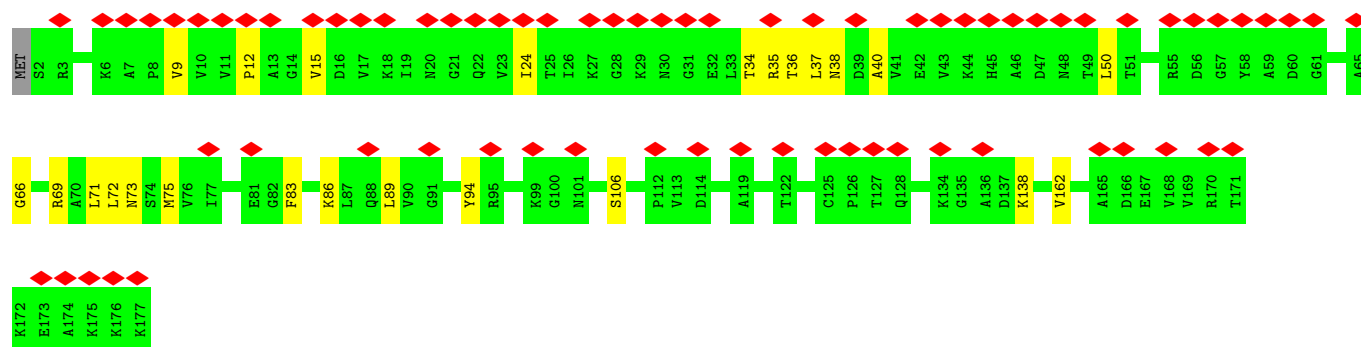
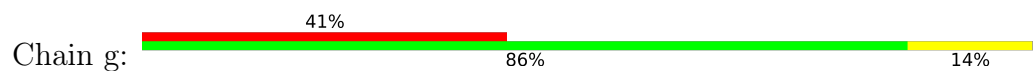


• Molecule 37: 50S ribosomal protein L5

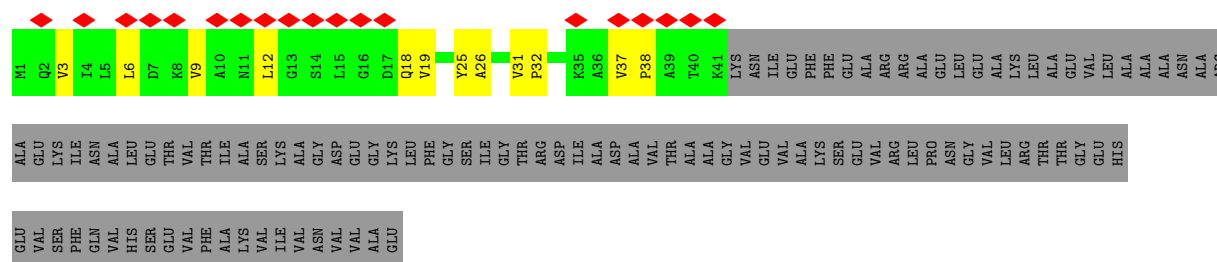




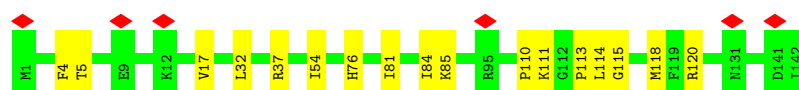
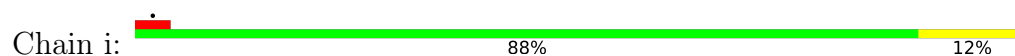
• Molecule 38: 50S ribosomal protein L6



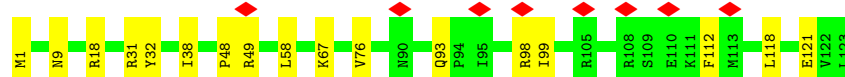
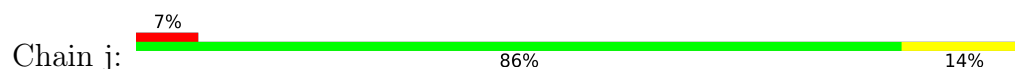
• Molecule 39: 50S ribosomal protein L9



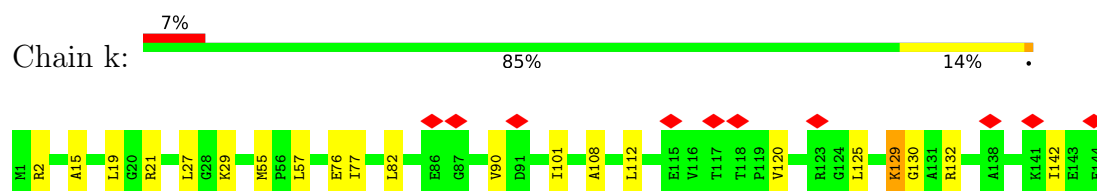
• Molecule 40: 50S ribosomal protein L13



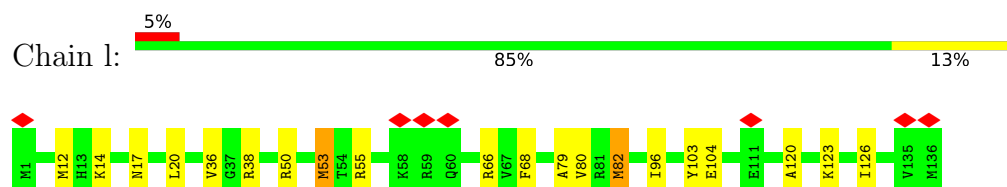
• Molecule 41: 50S ribosomal protein L14



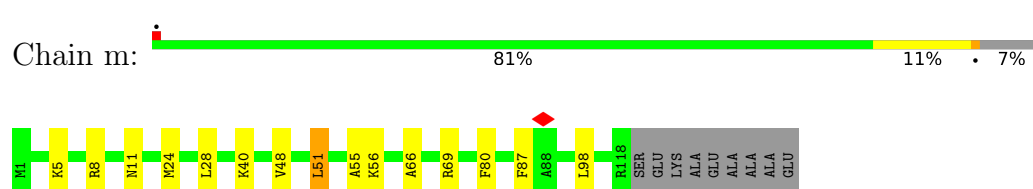
- Molecule 42: 50S ribosomal protein L15



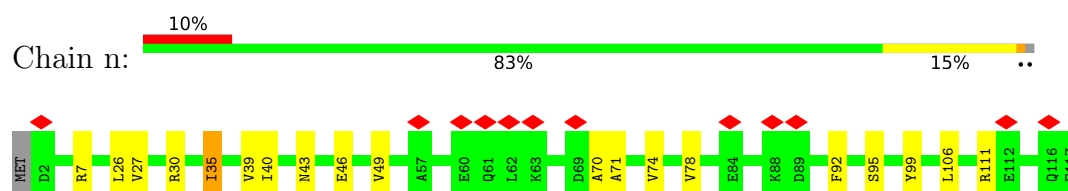
- Molecule 43: 50S ribosomal protein L16



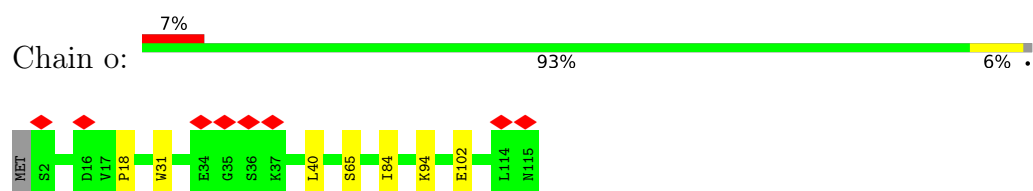
- Molecule 44: 50S ribosomal protein L17



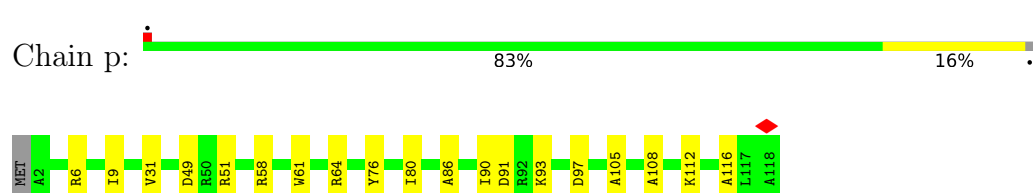
- Molecule 45: 50S ribosomal protein L18



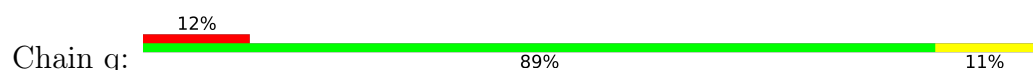
- Molecule 46: 50S ribosomal protein L19

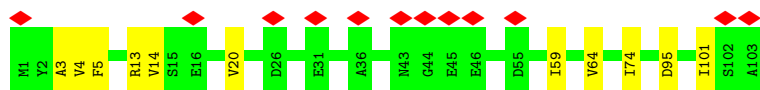


- Molecule 47: 50S ribosomal protein L20

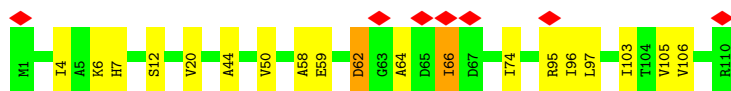
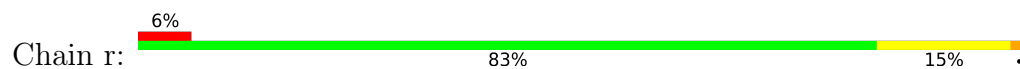


- Molecule 48: 50S ribosomal protein L21

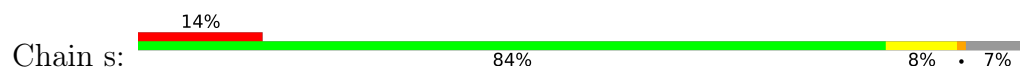




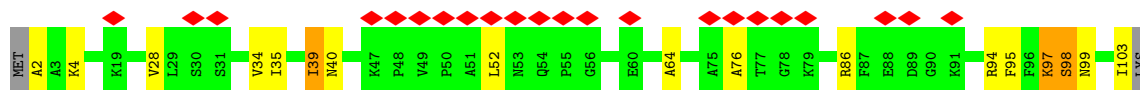
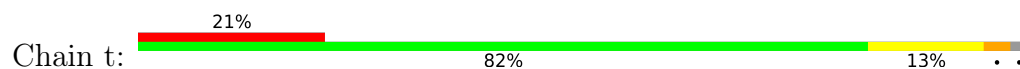
- Molecule 49: 50S ribosomal protein L22



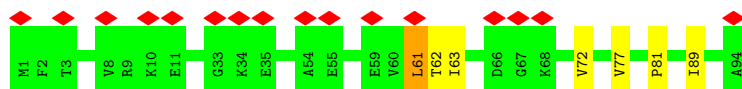
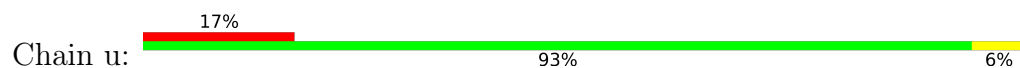
- Molecule 50: 50S ribosomal protein L23



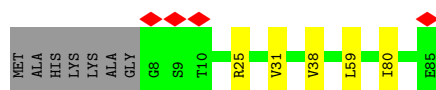
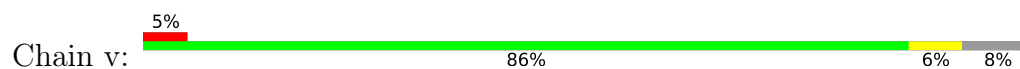
- Molecule 51: 50S ribosomal protein L24



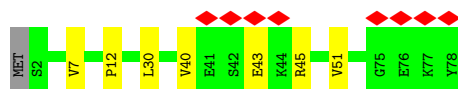
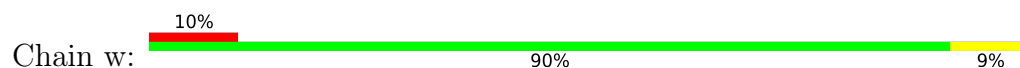
- Molecule 52: 50S ribosomal protein L25



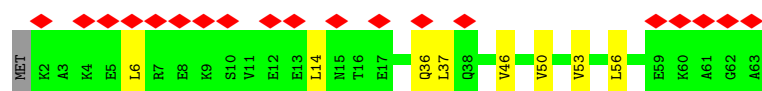
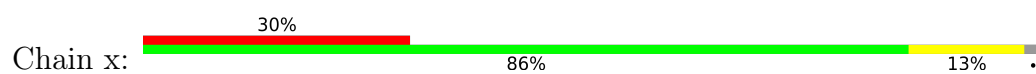
- Molecule 53: 50S ribosomal protein L27



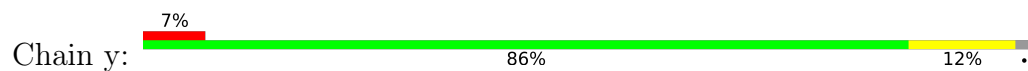
- Molecule 54: 50S ribosomal protein L28



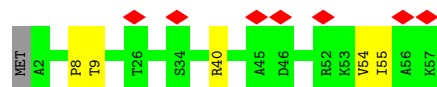
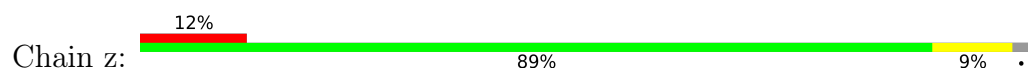
- Molecule 55: 50S ribosomal protein L29



- Molecule 56: 50S ribosomal protein L30



- Molecule 57: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137449	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, 4OC, PSU, SPM, 6MZ, G7M, UR3, H2U, OMG, 2MG, OMU, MG, 5MU, ZN, A2G, 2MA, 5MC, MEQ, OMC

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	0.41	0/424	0.73	0/565
2	1	0.48	0/380	0.83	0/498
3	2	0.44	0/513	0.81	0/676
4	3	0.45	0/303	0.75	0/397
5	4	0.40	0/488	0.74	0/649
6	A	0.82	0/162	1.04	0/221
7	B	0.53	1/36287 (0.0%)	0.92	26/56602 (0.0%)
8	C	1.01	0/1784	1.53	0/2403
9	D	0.98	0/1651	1.38	0/2225
10	E	0.98	0/1665	1.50	0/2227
11	F	1.00	0/1165	1.39	0/1568
12	G	1.04	1/858 (0.1%)	1.39	0/1160
13	H	1.01	0/1219	1.53	0/1635
14	I	1.00	0/989	1.39	0/1326
15	J	0.98	0/1034	1.46	0/1375
16	K	1.00	0/796	1.36	0/1077
17	L	1.00	0/893	1.38	0/1205
18	M	0.94	0/969	1.30	0/1300
19	N	1.00	0/900	1.56	0/1204
20	O	0.96	0/817	1.53	0/1088
21	P	0.94	0/722	1.55	0/964
22	Q	0.95	0/653	1.40	0/877
23	R	1.04	0/650	1.29	0/871
24	S	0.94	0/553	1.47	0/742
25	T	0.98	0/685	1.38	1/922 (0.1%)
26	U	0.97	0/676	1.72	0/895
27	V	0.95	0/597	1.54	0/792
28	W	0.97	0/2832	1.44	0/3816
29	X	0.86	0/1813	0.94	0/2823
30	Y	0.81	0/209	0.99	0/322
31	Z	0.87	0/1805	0.86	0/2812

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	a	0.82	9/65700 (0.0%)	1.00	64/102494 (0.1%)
33	b	0.82	0/2850	0.94	0/4444
34	c	0.94	0/2121	1.26	2/2852 (0.1%)
35	d	0.93	0/1576	1.35	0/2119
36	e	0.97	0/1571	1.42	0/2113
37	f	0.98	0/1434	1.45	3/1926 (0.2%)
38	g	1.03	0/1343	1.39	0/1816
39	h	1.06	0/306	1.35	0/413
40	i	0.91	0/1152	1.30	0/1551
41	j	0.94	0/955	1.31	0/1279
42	k	0.97	0/1062	1.39	2/1413 (0.1%)
43	l	0.90	0/1093	1.34	0/1460
44	m	0.91	0/958	1.42	0/1281
45	n	0.96	0/902	1.49	0/1209
46	o	0.93	0/929	1.24	0/1242
47	p	0.88	0/960	1.54	0/1278
48	q	0.95	0/829	1.21	0/1107
49	r	0.94	0/864	1.38	0/1156
50	s	0.97	0/744	1.34	0/994
51	t	1.01	0/787	1.36	0/1051
52	u	0.97	0/766	1.31	0/1025
53	v	0.93	0/593	1.29	0/785
54	w	0.90	0/635	1.34	0/848
55	x	0.94	0/502	1.58	0/667
56	y	0.97	0/453	1.37	0/605
57	z	0.94	0/450	1.36	0/599
All	All	0.81	11/156027 (0.0%)	1.10	98/232964 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	103	VAL	C-O	9.23	1.42	1.23
32	a	2069	G7M	O3'-P	5.65	1.61	1.56
32	a	2018	G	C5-C4	5.37	1.49	1.38
32	a	796	C	N1-C2	5.30	1.50	1.40
32	a	796	C	C4-C5	5.27	1.53	1.43
32	a	2018	G	N1-C2	5.19	1.48	1.37
32	a	2018	G	C2'-C1'	5.18	1.61	1.53
32	a	1846	G	C2'-C1'	5.18	1.61	1.53
32	a	1895	C	N1-C2	5.17	1.50	1.40
7	B	527	G7M	O3'-P	5.14	1.61	1.56
32	a	683	U	C1'-N1	5.13	1.56	1.48

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	329	G	O3'-P-O5'	-8.84	90.74	104.00
32	a	827	U	C2'-C3'-O3'	-7.29	102.76	113.70
7	B	976	G	O3'-P-O5'	-7.26	93.11	104.00
7	B	561	U	O3'-P-O5'	-7.25	93.12	104.00
32	a	2030	A	C2'-C3'-O3'	7.14	120.20	109.50
32	a	1606	C	C2'-C3'-O3'	-6.97	103.25	113.70
34	c	151	GLY	CA-C-O	-6.47	118.01	122.22
32	a	1565	C	O3'-P-O5'	-6.40	94.40	104.00
32	a	204	A	O3'-P-O5'	-6.37	94.45	104.00
32	a	1913	A	P-O3'-C3'	-6.30	110.75	120.20
32	a	1915	U	P-O3'-C3'	-6.30	110.75	120.20
32	a	2884	U	O3'-P-O5'	-6.29	94.57	104.00
32	a	784	G	C2'-C3'-O3'	-6.26	104.31	113.70
32	a	2030	A	O3'-P-O5'	6.25	113.37	104.00
34	c	234	GLY	CA-C-O	-6.22	117.97	122.45
32	a	1971	U	C2'-C3'-O3'	-6.19	104.41	113.70
32	a	2346	A	O3'-P-O5'	-6.19	94.72	104.00
32	a	621	A	O3'-P-O5'	-6.13	94.80	104.00
32	a	2050	C	O3'-P-O5'	-6.08	94.87	104.00
32	a	1377	G	O3'-P-O5'	-6.06	94.91	104.00
7	B	935	A	O3'-P-O5'	-6.06	94.92	104.00
7	B	159	G	O3'-P-O5'	-6.03	94.96	104.00
32	a	781	A	C4'-C3'-O3'	-6.02	103.98	113.00
7	B	348	G	O3'-P-O5'	-6.01	94.99	104.00
7	B	181	A	O3'-P-O5'	-6.00	95.00	104.00
37	f	107	ALA	CA-C-N	5.97	125.11	120.33
37	f	107	ALA	C-N-CA	5.97	125.11	120.33
32	a	2820	A	C2'-C3'-O3'	5.96	118.45	109.50
32	a	1638	C	O3'-P-O5'	-5.94	95.09	104.00
7	B	720	C	C4'-C3'-O3'	-5.93	104.11	113.00
32	a	2566	A	O3'-P-O5'	-5.88	95.18	104.00
32	a	1914	C	P-O3'-C3'	-5.88	111.38	120.20
32	a	1966	A	O3'-P-O5'	-5.84	95.24	104.00
7	B	126	G	O3'-P-O5'	-5.77	95.34	104.00
32	a	2060	A	O3'-P-O5'	-5.76	95.36	104.00
32	a	2050	C	C4'-C3'-O3'	-5.75	104.38	113.00
32	a	2477	U	O3'-P-O5'	-5.74	95.39	104.00
32	a	1185	G	O3'-P-O5'	-5.72	95.42	104.00
7	B	1220	G	O3'-P-O5'	-5.72	95.43	104.00
32	a	1825	U	O3'-P-O5'	-5.70	95.45	104.00
32	a	825	A	O3'-P-O5'	-5.68	95.48	104.00
7	B	57	G	O3'-P-O5'	-5.67	95.49	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	765	G	O3'-P-O5'	-5.66	95.51	104.00
32	a	124	G	O3'-P-O5'	-5.61	95.58	104.00
32	a	828	U	C4'-C3'-O3'	-5.57	104.64	113.00
7	B	1103	C	O3'-P-O5'	-5.56	95.67	104.00
32	a	158	U	P-O3'-C3'	-5.49	111.97	120.20
7	B	239	U	C2'-C3'-O3'	-5.49	105.47	113.70
7	B	455	G	O3'-P-O5'	-5.49	95.77	104.00
32	a	1194	A	O3'-P-O5'	-5.48	95.77	104.00
32	a	1254	A	C4'-C3'-O3'	-5.48	104.77	113.00
32	a	2237	G	O3'-P-O5'	-5.48	95.78	104.00
7	B	1201	A	O3'-P-O5'	-5.46	95.80	104.00
32	a	2817	U	O3'-P-O5'	-5.46	95.81	104.00
32	a	2519	U	O3'-P-O5'	-5.45	95.82	104.00
7	B	652	U	O3'-P-O5'	-5.42	95.86	104.00
32	a	2620	C	O3'-P-O5'	-5.40	95.90	104.00
32	a	2001	C	O3'-P-O5'	-5.37	95.94	104.00
32	a	2820	A	C4'-C3'-O3'	-5.35	101.37	109.40
32	a	2382	G	O3'-P-O5'	-5.35	95.97	104.00
32	a	959	A	C4'-C3'-O3'	-5.35	104.98	113.00
32	a	1905	C	O3'-P-O5'	-5.34	95.99	104.00
32	a	1778	U	O3'-P-O5'	-5.34	96.00	104.00
37	f	116	GLY	CA-C-O	-5.33	118.31	122.52
32	a	2428	G	C2'-C3'-O3'	-5.32	105.72	113.70
32	a	781	A	O3'-P-O5'	-5.30	96.04	104.00
32	a	2278	A	O3'-P-O5'	-5.29	96.06	104.00
32	a	1133	A	O3'-P-O5'	-5.28	96.08	104.00
7	B	1377	A	O3'-P-O5'	-5.28	96.08	104.00
32	a	1785	A	O3'-P-O5'	-5.27	96.09	104.00
32	a	2079	U	O3'-P-O5'	-5.26	96.11	104.00
32	a	2882	A	O3'-P-O5'	-5.25	96.12	104.00
32	a	2449	H2U	O3'-P-O5'	-5.24	96.14	104.00
7	B	8	A	O3'-P-O5'	-5.22	96.17	104.00
32	a	2378	A	O3'-P-O5'	-5.21	96.18	104.00
32	a	2208	C	P-O3'-C3'	-5.19	112.42	120.20
7	B	1235	U	O3'-P-O5'	-5.16	96.25	104.00
32	a	726	G	O3'-P-O5'	-5.16	96.26	104.00
42	k	15	ALA	CA-C-N	5.15	124.99	120.10
42	k	15	ALA	C-N-CA	5.15	124.99	120.10
32	a	242	G	C3'-C2'-C1'	-5.14	96.36	101.50
7	B	297	G	O3'-P-O5'	-5.12	96.32	104.00
32	a	1697	G	O3'-P-O5'	-5.11	96.33	104.00
32	a	1235	G	C2'-C3'-O3'	-5.11	106.04	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	604	G	O3'-P-O5'	-5.10	96.35	104.00
7	B	572	A	O3'-P-O5'	-5.07	96.40	104.00
32	a	513	A	O3'-P-O5'	-5.06	96.40	104.00
32	a	450	G	O3'-P-O5'	-5.05	96.42	104.00
7	B	378	G	O3'-P-O5'	-5.04	96.43	104.00
32	a	2622	U	O3'-P-O5'	-5.04	96.44	104.00
7	B	150	U	O3'-P-O5'	-5.03	96.45	104.00
7	B	877	G	O3'-P-O5'	-5.03	96.46	104.00
25	T	82	GLY	CA-C-O	-5.03	118.70	122.37
32	a	2756	U	C4'-C3'-O3'	5.03	116.94	109.40
7	B	977	A	O3'-P-O5'	-5.02	96.47	104.00
32	a	856	G	O3'-P-O5'	-5.01	96.48	104.00
32	a	1969	A	O3'-P-O5'	-5.01	96.48	104.00
7	B	921	U	O3'-P-O5'	-5.01	96.48	104.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	4	0
2	1	377	0	418	3	0
3	2	504	0	572	5	0
4	3	302	0	340	1	0
5	4	480	0	478	4	0
6	A	155	0	164	5	0
7	B	32608	0	16424	122	0
8	C	1753	0	1780	27	0
9	D	1624	0	1696	15	0
10	E	1643	0	1707	29	0
11	F	1152	0	1196	18	0
12	G	839	0	833	20	0
13	H	1203	0	1254	12	0
14	I	979	0	1031	22	0
15	J	1022	0	1070	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	786	0	828	9	0
17	L	877	0	887	13	0
18	M	955	0	1016	11	0
19	N	891	0	952	14	0
20	O	805	0	844	9	0
21	P	714	0	734	3	0
22	Q	643	0	661	12	0
23	R	641	0	682	8	0
24	S	544	0	565	7	0
25	T	668	0	693	4	0
26	U	670	0	719	7	0
27	V	589	0	629	3	0
28	W	2792	0	2723	31	0
29	X	1623	0	821	6	0
30	Y	188	0	96	0	0
31	Z	1616	0	821	2	0
32	a	59128	0	29763	229	0
33	b	2549	0	1291	6	0
34	c	2082	0	2154	22	0
35	d	1566	0	1618	16	0
36	e	1552	0	1619	17	0
37	f	1410	0	1444	18	0
38	g	1323	0	1371	13	0
39	h	303	0	327	6	0
40	i	1129	0	1162	12	0
41	j	946	0	1023	11	0
42	k	1053	0	1129	18	0
43	l	1074	0	1157	14	0
44	m	945	0	989	9	0
45	n	892	0	923	13	0
46	o	917	0	962	6	0
47	p	947	0	1019	14	0
48	q	816	0	839	7	0
49	r	857	0	922	10	0
50	s	738	0	807	5	0
51	t	779	0	831	8	0
52	u	753	0	780	5	0
53	v	586	0	596	3	0
54	w	625	0	652	4	0
55	x	501	0	531	3	0
56	y	449	0	488	4	0
57	z	444	0	458	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	3	1	0	0	0	0
58	4	1	0	0	0	0
59	A	14	0	12	0	0
60	B	89	0	0	0	0
60	a	208	0	0	0	0
60	b	5	0	0	0	0
60	c	1	0	0	0	0
60	d	1	0	0	0	0
60	z	1	0	0	0	0
61	a	14	0	26	2	0
62	0	1	0	0	0	0
62	1	2	0	0	0	0
62	2	12	0	0	0	0
62	3	3	0	0	0	0
62	A	16	0	0	0	0
62	B	189	0	0	1	0
62	D	2	0	0	0	0
62	E	1	0	0	0	0
62	F	2	0	0	0	0
62	M	2	0	0	0	0
62	N	1	0	0	0	0
62	R	1	0	0	0	0
62	W	18	0	0	0	0
62	X	1	0	0	0	0
62	Y	6	0	0	0	0
62	a	1331	0	0	3	0
62	b	10	0	0	0	0
62	c	41	0	0	0	0
62	d	20	0	0	0	0
62	e	15	0	0	0	0
62	h	1	0	0	0	0
62	i	2	0	0	1	0
62	j	5	0	0	0	0
62	k	16	0	0	1	0
62	l	8	0	0	0	0
62	m	8	0	0	0	0
62	n	1	0	0	0	0
62	o	5	0	0	0	0
62	p	8	0	0	0	0
62	q	3	0	0	0	0
62	r	7	0	0	0	0
62	s	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	t	1	0	0	0	0
62	u	1	0	0	0	0
62	v	3	0	0	0	0
62	w	3	0	0	0	0
62	z	7	0	0	0	0
All	All	146513	0	97978	800	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 (800) 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)
32:a:1618:6MZ:N6	32:a:1618:6MZ:C9	1.68	1.52
43:l:66:ARG:NH1	43:l:104:GLU:OE2	2.08	0.86
11:F:115:LEU:HD13	11:F:123:VAL:HG11	1.58	0.84
11:F:115:LEU:HD22	11:F:120:VAL:HG21	1.57	0.84
15:J:52:LEU:HD11	15:J:63:LEU:HD11	1.58	0.83
32:a:12:U:H2'	32:a:12:U:O2	1.78	0.82
42:k:108:ALA:HB3	42:k:125:LEU:HD22	1.62	0.81
32:a:1618:6MZ:C9	32:a:1618:6MZ:C6	2.59	0.80
10:E:107:PHE:CD1	10:E:145:ILE:HD11	2.17	0.80
7:B:664:G:H22	7:B:741:G:H1	1.33	0.75
3:2:12:LYS:NZ	32:a:249:C:O2	2.19	0.74
32:a:2453:A:OP1	62:a:6301:HOH:O	2.05	0.74
14:I:11:LEU:HD22	14:I:75:ILE:HD11	1.69	0.74
9:D:149:ILE:CD1	9:D:202:ILE:HD13	2.18	0.74
15:J:84:THR:HG23	15:J:98:LEU:HD13	1.68	0.73
44:m:66:ALA:O	44:m:69:ARG:O	2.05	0.73
51:t:28:VAL:HG22	51:t:34:VAL:HG12	1.71	0.73
45:n:39:VAL:HB	45:n:49:VAL:HG22	1.71	0.73
18:M:80:ILE:HD12	18:M:97:THR:HG22	1.71	0.72
43:l:20:LEU:HD13	52:u:81:PRO:HG2	1.70	0.71
3:2:54:ASP:HB3	42:k:57:LEU:HD22	1.71	0.71
7:B:1328:C:H5''	19:N:28:THR:HG21	1.72	0.71
34:c:29:PRO:HG2	34:c:34:LEU:HD11	1.71	0.71
43:l:53:MET:HE1	43:l:103:TYR:CD2	2.26	0.71
38:g:89:LEU:HD22	38:g:162:VAL:HG22	1.72	0.71
32:a:930:G:H1'	56:y:25:LEU:HD11	1.72	0.70
19:N:39:ILE:HD12	19:N:56:LEU:HD21	1.73	0.70
28:W:226:THR:HG22	28:W:244:ILE:HD13	1.76	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:111:LEU:HD11	9:D:146:ALA:HB2	1.75	0.68
10:E:145:ILE:HD12	10:E:178:MET:HB3	1.76	0.68
34:c:142:HIS:ND1	34:c:193:GLY:O	2.27	0.68
10:E:145:ILE:HD13	10:E:155:VAL:HG11	1.76	0.68
7:B:945:G:C2	7:B:946:A:C8	2.81	0.68
45:n:27:VAL:HG21	45:n:40:ILE:HD12	1.75	0.67
7:B:677:U:H3	7:B:713:G:H22	1.41	0.67
19:N:33:ILE:HD13	19:N:60:VAL:HG22	1.76	0.67
32:a:757:G:N7	62:a:6303:HOH:O	2.27	0.67
22:Q:4:ILE:HG12	22:Q:21:VAL:HG22	1.77	0.67
40:i:76:HIS:CE1	40:i:85:LYS:HB2	2.30	0.67
55:x:6:LEU:HD23	55:x:53:VAL:HG22	1.77	0.66
28:W:115:VAL:HG22	28:W:203:VAL:HG22	1.78	0.66
16:K:66:GLU:HB2	20:O:99:ALA:HB2	1.78	0.65
19:N:40:ALA:HB3	19:N:43:VAL:HG23	1.77	0.65
10:E:145:ILE:HD13	10:E:155:VAL:CG1	2.26	0.65
34:c:133:ARG:HB3	34:c:186:ALA:HB1	1.79	0.64
32:a:1799:G:O2'	34:c:180:GLU:OE2	2.09	0.64
32:a:1939:5MU:OP1	32:a:2604:PSU:O2'	2.14	0.64
22:Q:3:THR:HG22	22:Q:66:THR:OG1	1.96	0.64
28:W:134:MET:SD	28:W:337:LEU:HD21	2.38	0.64
22:Q:57:ILE:HD13	22:Q:75:ILE:HD11	1.79	0.64
10:E:57:GLU:CG	10:E:199:LEU:HD12	2.28	0.63
21:P:25:THR:HG21	21:P:70:LEU:HB2	1.80	0.63
7:B:1526:G:N7	27:V:40:LYS:NZ	2.46	0.63
7:B:407:U:O2'	10:E:113:GLU:OE2	2.17	0.63
32:a:811:U:H2'	42:k:21:ARG:HA	1.81	0.62
37:f:30:ARG:H	37:f:159:THR:HG1	1.47	0.62
9:D:149:ILE:HD13	9:D:202:ILE:HD13	1.81	0.62
14:I:10:MET:HG3	14:I:27:MET:HE2	1.81	0.62
35:d:25:THR:HG21	35:d:193:VAL:HG22	1.80	0.61
36:e:184:ASP:HA	42:k:2:ARG:HH12	1.65	0.61
1:O:22:THR:HG21	32:a:2419:U:H4'	1.81	0.61
18:M:33:VAL:HG22	18:M:79:VAL:HG22	1.81	0.61
7:B:769:G:H4'	7:B:1513:A:H4'	1.81	0.61
15:J:88:MET:HE2	15:J:104:VAL:HG22	1.82	0.61
32:a:1754:A:N1	32:a:2716:C:O2'	2.33	0.61
37:f:50:LEU:HD11	37:f:67:ILE:HD12	1.83	0.61
12:G:10:VAL:HG21	12:G:18:VAL:HG22	1.83	0.60
32:a:2780:G:OP2	40:i:120:ARG:HD3	2.00	0.60
10:E:57:GLU:HG3	10:E:199:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:24:ILE:HD13	37:f:106:ILE:CD1	2.32	0.60
8:C:162:PHE:CE2	8:C:164:ILE:HD11	2.37	0.60
15:J:19:VAL:HG22	15:J:65:ILE:HG12	1.84	0.60
7:B:160:A:H2'	7:B:161:A:O4'	2.01	0.60
57:z:54:VAL:HG23	57:z:55:ILE:HG23	1.82	0.60
41:j:121:GLU:OE1	46:o:65:SER:OG	2.18	0.59
17:L:113:VAL:HG12	24:S:73:ARG:HD2	1.83	0.59
43:l:53:MET:HG3	43:l:120:ALA:HB2	1.83	0.59
28:W:255:VAL:HG11	28:W:274:LEU:HB2	1.84	0.59
11:F:115:LEU:HB3	11:F:120:VAL:HG23	1.84	0.59
7:B:1402:4OC:O2	7:B:1500:A:N1	2.35	0.59
20:O:89:MET:HA	20:O:89:MET:HE2	1.82	0.59
32:a:1020:A:C2	32:a:1141:U:C2	2.91	0.59
7:B:946:A:H2'	7:B:947:G:C8	2.37	0.59
7:B:977:A:O2'	7:B:979:C:OP2	2.21	0.59
15:J:88:MET:CE	15:J:104:VAL:HG22	2.33	0.59
32:a:2018:G:OP1	62:a:6302:HOH:O	2.17	0.59
12:G:29:ILE:HG21	12:G:64:VAL:HG13	1.84	0.58
51:t:94:ARG:HB3	51:t:103:ILE:HD12	1.85	0.58
7:B:543:U:OP1	10:E:14:ARG:HD2	2.03	0.58
8:C:14:VAL:HG13	8:C:213:TYR:OH	2.04	0.58
26:U:28:MET:HE1	26:U:67:ILE:HG21	1.86	0.58
37:f:50:LEU:CD1	37:f:67:ILE:HD12	2.34	0.58
49:r:4:ILE:HG12	49:r:106:VAL:HG22	1.85	0.58
38:g:9:VAL:HG13	38:g:69:ARG:NE	2.19	0.57
44:m:8:ARG:HH11	44:m:8:ARG:HG3	1.69	0.57
10:E:154:ARG:HG3	10:E:154:ARG:HH11	1.70	0.57
14:I:10:MET:HA	14:I:27:MET:HE2	1.86	0.57
40:i:32:LEU:CD2	40:i:54:ILE:HG21	2.35	0.57
32:a:543:G:H1	32:a:550:C:H42	1.52	0.57
51:t:39:ILE:HG22	51:t:40:ASN:N	2.19	0.57
8:C:27:MET:HE2	8:C:187:VAL:HG12	1.87	0.57
28:W:137:ARG:HH11	28:W:137:ARG:HB3	1.69	0.57
32:a:2205:A:H61	32:a:2219:U:H3	1.53	0.57
42:k:77:ILE:HD12	42:k:77:ILE:N	2.20	0.57
32:a:729:G:C6	34:c:207:LYS:HB2	2.40	0.56
29:X:16:U:O2'	29:X:17:C:OP1	2.22	0.56
2:1:39:ARG:NH2	32:a:468:G:N7	2.49	0.56
32:a:2038:G:H2'	32:a:2039:U:O4'	2.05	0.56
8:C:151:ILE:HG23	8:C:154:MET:HE2	1.88	0.56
52:u:63:ILE:HD12	52:u:72:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:12:U:O2	32:a:12:U:C2'	2.53	0.56
7:B:451:A:H61	7:B:481:G:H5'	1.70	0.56
32:a:2020:A:H5'	57:z:9:THR:CG2	2.36	0.56
32:a:2547:A:H2'	32:a:2548:U:C6	2.40	0.56
54:w:12:PRO:HB3	54:w:30:LEU:HD23	1.87	0.56
37:f:44:ILE:HG21	37:f:79:ILE:HG22	1.86	0.56
42:k:76:GLU:C	42:k:77:ILE:HD12	2.30	0.56
35:d:156:PHE:CE1	40:i:81:ILE:HD13	2.41	0.55
43:l:96:ILE:HG21	43:l:126:ILE:HD12	1.88	0.55
53:v:25:ARG:HH11	53:v:31:VAL:HG12	1.70	0.55
32:a:1421:G:C2	32:a:1422:G:C8	2.94	0.55
7:B:1422:G:O3'	41:j:49:ARG:NH1	2.38	0.55
22:Q:52:LEU:HD12	22:Q:78:VAL:HG21	1.88	0.55
32:a:2748:A:O2'	38:g:66:GLY:HA3	2.07	0.55
25:T:80:TYR:CZ	25:T:82:GLY:HA2	2.41	0.55
38:g:69:ARG:HG3	38:g:69:ARG:HH11	1.72	0.55
34:c:4:VAL:HG13	34:c:18:LYS:HG3	1.89	0.55
18:M:4:VAL:HG23	23:R:34:TYR:HB3	1.89	0.55
32:a:2506:U:C2	32:a:2585:U:O4	2.60	0.55
7:B:411:A:P	10:E:26:ARG:HH22	2.30	0.54
23:R:64:CYS:SG	23:R:74:THR:HG23	2.46	0.54
32:a:1881:C:H2'	32:a:1882:U:O4'	2.06	0.54
35:d:12:THR:HG22	35:d:13:ARG:H	1.71	0.54
7:B:181:A:N6	7:B:195:A:C8	2.76	0.54
42:k:77:ILE:HD13	42:k:108:ALA:HB1	1.87	0.54
17:L:114:THR:HG21	27:V:32:VAL:HG21	1.89	0.54
28:W:177:PHE:O	28:W:321:ARG:NH2	2.40	0.54
32:a:1182:G:H2'	32:a:1183:U:O4'	2.08	0.54
10:E:130:VAL:HG11	10:E:135:TYR:CD2	2.43	0.54
42:k:19:LEU:HD23	42:k:27:LEU:HD13	1.89	0.54
32:a:1721:G:N2	32:a:1738:G:O2'	2.40	0.54
51:t:4:LYS:O	51:t:94:ARG:NH2	2.41	0.54
14:I:66:PHE:CD2	14:I:67:GLN:HG2	2.42	0.54
32:a:534:U:O2'	47:p:49:ASP:OD2	2.22	0.54
32:a:1799:G:N7	34:c:178:SER:OG	2.37	0.54
32:a:2093:G:O2'	32:a:2198:A:N1	2.38	0.53
32:a:2627:G:O2'	32:a:2781:A:N1	2.32	0.53
44:m:56:LYS:HE2	44:m:87:PHE:O	2.08	0.53
49:r:58:ALA:O	49:r:62:ASP:O	2.27	0.53
21:P:24:SER:OG	21:P:27:VAL:HG23	2.09	0.53
28:W:319:ASP:OD2	28:W:344:ILE:HD11	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:100:MET:HE2	8:C:151:ILE:HD12	1.91	0.53
32:a:1125:G:C6	32:a:1126:A:N6	2.76	0.53
7:B:1067:A:N1	7:B:1108:G:O2'	2.37	0.53
13:H:69:VAL:HG21	13:H:104:ILE:HD11	1.89	0.53
14:I:104:VAL:HG22	14:I:125:ILE:HD13	1.91	0.53
34:c:155:ALA:HB2	34:c:162:VAL:HG23	1.91	0.53
49:r:58:ALA:O	49:r:64:ALA:HB3	2.08	0.53
9:D:149:ILE:HD12	9:D:202:ILE:HD13	1.91	0.53
37:f:100:PHE:CZ	37:f:104:ILE:HD11	2.44	0.53
2:l:29:GLN:NE2	32:a:210:C:OP1	2.37	0.53
12:G:90:MET:HE1	24:S:23:TYR:CZ	2.44	0.53
42:k:21:ARG:N	62:k:201:HOH:O	2.39	0.53
11:F:81:LEU:HD22	11:F:147:MET:HE1	1.91	0.52
11:F:153:VAL:HG21	14:I:99:LEU:HD13	1.91	0.52
32:a:2243:U:H2'	32:a:2244:U:C6	2.44	0.52
43:l:82:MET:HA	43:l:82:MET:CE	2.39	0.52
7:B:927:G:O2'	7:B:1503:A:N7	2.37	0.52
11:F:97:GLN:HE21	11:F:124:LEU:HD12	1.73	0.52
18:M:4:VAL:CG2	23:R:34:TYR:HB3	2.40	0.52
32:a:819:A:C4	32:a:1189:A:C2	2.98	0.52
47:p:76:TYR:CZ	47:p:80:ILE:HG13	2.44	0.52
7:B:403:C:H2'	7:B:404:G:H5''	1.92	0.52
32:a:1320:C:N3	32:a:1331:G:O6	2.43	0.52
33:b:42:C:C5	37:f:66:LEU:HD22	2.45	0.52
47:p:86:ALA:HB2	47:p:116:ALA:HB2	1.91	0.52
7:B:574:A:OP2	62:B:1701:HOH:O	2.19	0.52
26:U:42:GLY:HA2	26:U:86:LEU:HD11	1.90	0.52
32:a:1570:A:H2'	32:a:1571:A:C8	2.45	0.52
32:a:1964:G:H4'	32:a:1965:C:OP2	2.09	0.52
7:B:1394:A:N1	7:B:1500:A:O2'	2.41	0.52
15:J:19:VAL:HG22	15:J:65:ILE:HG23	1.91	0.51
19:N:77:ILE:HG22	19:N:81:MET:HE2	1.91	0.51
25:T:15:LEU:HD12	25:T:38:SER:CB	2.40	0.51
7:B:404:G:H5''	7:B:404:G:H8	1.76	0.51
32:a:2000:C:OP1	44:m:5:LYS:NZ	2.28	0.51
32:a:588:U:H2'	32:a:589:U:C6	2.45	0.51
50:s:48:GLN:HE21	50:s:55:VAL:H	1.58	0.51
12:G:26:THR:HG22	12:G:36:ILE:HD13	1.91	0.51
32:a:695:G:O6	61:a:6209:SPM:H122	2.10	0.51
36:e:23:PHE:CD1	36:e:111:GLU:HG3	2.46	0.51
1:O:54:ILE:HG21	32:a:2420:C:H4'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:6:TYR:O	36:e:61:ARG:NH1	2.40	0.51
22:Q:57:ILE:HG21	22:Q:75:ILE:HD11	1.93	0.51
7:B:519:C:H2'	7:B:520:A:O4'	2.11	0.51
43:l:50:ARG:HA	43:l:53:MET:HE2	1.93	0.51
45:n:43:ASN:HD21	45:n:46:GLU:HG2	1.75	0.51
16:K:54:SER:O	20:O:81:ARG:NH1	2.39	0.51
14:I:13:ARG:HD2	14:I:27:MET:HE3	1.93	0.51
16:K:10:LEU:HB3	16:K:18:ILE:HD11	1.93	0.51
32:a:614:A:H3'	32:a:615:U:C5'	2.41	0.51
7:B:1103:C:O2	8:C:106:THR:HG21	2.11	0.51
10:E:170:TRP:CD2	10:E:186:PRO:HB3	2.46	0.51
7:B:933:G:P	13:H:4:ARG:HH12	2.33	0.50
7:B:1225:A:H2'	7:B:1225:A:N3	2.26	0.50
12:G:18:VAL:HG21	12:G:58:HIS:ND1	2.26	0.50
15:J:43:THR:O	15:J:47:VAL:HG23	2.10	0.50
32:a:2312:U:H5'	37:f:85:ILE:HD11	1.93	0.50
7:B:337:G:H2'	7:B:338:A:C8	2.46	0.50
29:X:52:G:H1	29:X:62:C:H42	1.57	0.50
32:a:1932:A:H2'	32:a:1933:G:O4'	2.12	0.50
32:a:2395:C:H2'	32:a:2396:G:O4'	2.11	0.50
32:a:2443:C:OP1	36:e:63:LYS:HD3	2.12	0.50
37:f:8:TYR:O	37:f:13:VAL:HG23	2.11	0.50
7:B:718:A:H5'	17:L:119:ASN:CG	2.37	0.50
7:B:909:A:H2'	7:B:910:C:O4'	2.10	0.50
32:a:493:G:H2'	32:a:494:G:O4'	2.10	0.50
36:e:48:THR:HG23	36:e:88:ARG:NH1	2.26	0.50
49:r:74:ILE:HG13	49:r:105:VAL:HG22	1.94	0.50
2:l:1:MET:SD	32:a:752:A:H3'	2.52	0.50
7:B:860:A:H2'	7:B:861:G:O4'	2.12	0.50
32:a:340:A:H2'	32:a:341:C:O4'	2.12	0.50
38:g:9:VAL:HG23	38:g:50:LEU:HB2	1.93	0.50
11:F:75:ALA:O	11:F:147:MET:HE3	2.11	0.50
32:a:693:A:N6	61:a:6209:SPM:H132	2.27	0.50
32:a:828:U:H2'	32:a:829:A:C8	2.47	0.50
32:a:1020:A:N1	32:a:1141:U:O2'	2.33	0.50
32:a:2483:C:N3	43:l:123:LYS:NZ	2.51	0.50
7:B:900:A:H2'	7:B:901:A:C8	2.47	0.50
22:Q:4:ILE:HG22	22:Q:71:VAL:HG11	1.94	0.50
42:k:77:ILE:CD1	42:k:108:ALA:HB1	2.41	0.50
7:B:1144:G:N2	7:B:1146:A:H62	2.10	0.50
34:c:76:ALA:HB3	34:c:116:ILE:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:f:2:ALA:HB1	37:f:5:HIS:HB3	1.93	0.50
38:g:35:ARG:NE	38:g:71:LEU:HD13	2.27	0.50
52:u:63:ILE:CD1	52:u:72:VAL:HG21	2.42	0.50
7:B:1424:U:H2'	7:B:1425:U:O4'	2.12	0.50
14:I:96:MET:SD	14:I:130:ALA:HB1	2.52	0.50
19:N:17:ILE:O	19:N:20:THR:OG1	2.23	0.50
21:P:29:VAL:HG11	21:P:67:LEU:HD21	1.94	0.50
24:S:32:TYR:HB3	24:S:55:LEU:HD21	1.93	0.50
32:a:1027:A:C6	32:a:1126:A:C4	2.99	0.50
17:L:113:VAL:HG12	24:S:73:ARG:CD	2.42	0.49
7:B:1317:C:O5'	20:O:24:ARG:NH2	2.45	0.49
32:a:2376:A:N3	45:n:111:ARG:NH1	2.60	0.49
45:n:30:ARG:HG3	45:n:35:ILE:HD12	1.94	0.49
28:W:179:SER:HA	28:W:203:VAL:O	2.12	0.49
32:a:1198:U:H5'	47:p:9:ILE:HD11	1.95	0.49
32:a:1944:U:C5	32:a:1955:U:C2	3.00	0.49
38:g:89:LEU:CD2	38:g:162:VAL:HG22	2.42	0.49
9:D:134:MET:HE2	9:D:168:TYR:CD2	2.48	0.49
9:D:148:GLY:HA3	9:D:172:ARG:O	2.12	0.49
13:H:26:PHE:HZ	13:H:120:LEU:HD11	1.77	0.49
34:c:91:ILE:HD12	34:c:103:TYR:CD1	2.48	0.49
48:q:5:PHE:HB3	48:q:59:ILE:HD12	1.92	0.49
12:G:90:MET:SD	24:S:61:ARG:NH1	2.86	0.49
14:I:39:VAL:HG21	14:I:110:VAL:HG12	1.94	0.49
19:N:52:GLN:O	19:N:55:THR:OG1	2.24	0.49
7:B:3:A:N1	7:B:628:G:O2'	2.46	0.49
10:E:37:ALA:HB1	10:E:38:PRO:CD	2.43	0.49
19:N:90:ARG:HD3	19:N:96:PRO:O	2.13	0.49
32:a:374:A:C2	32:a:401:A:C4	3.00	0.49
7:B:429:U:H3'	10:E:9:LEU:HD12	1.94	0.49
7:B:502:A:H2'	7:B:503:C:O4'	2.13	0.49
8:C:97:LEU:O	8:C:100:MET:HG3	2.12	0.49
9:D:14:ILE:HG22	9:D:15:VAL:HG13	1.93	0.49
12:G:66:ALA:HB1	12:G:67:PRO:HD2	1.95	0.49
29:X:8:U:O2'	29:X:21:A:N1	2.44	0.49
32:a:2823:A:C5	32:a:2824:C:C5	3.01	0.49
38:g:9:VAL:HG11	38:g:73:ASN:HB2	1.95	0.49
41:j:99:ILE:HD13	41:j:118:LEU:HB2	1.94	0.49
31:Z:75:C:O4'	32:a:2432:A:H1'	2.13	0.49
35:d:110:THR:CG2	35:d:202:ILE:HB	2.42	0.49
51:t:86:ARG:HG3	51:t:95:PHE:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:38:VAL:HG11	11:F:114:VAL:HG22	1.95	0.48
13:H:135:VAL:HG22	13:H:135:VAL:O	2.13	0.48
22:Q:57:ILE:HG21	22:Q:75:ILE:CD1	2.43	0.48
32:a:2636:C:HO2'	35:d:45:TYR:HH	1.60	0.48
48:q:64:VAL:HG22	48:q:95:ASP:O	2.12	0.48
16:K:52:LEU:HB2	20:O:81:ARG:HD2	1.94	0.48
36:e:149:ILE:HG22	36:e:192:ALA:HB1	1.94	0.48
7:B:176:C:H2'	7:B:177:G:N3	2.28	0.48
7:B:1356:G:H2'	7:B:1357:A:C8	2.49	0.48
9:D:175:LEU:HD21	9:D:201:TRP:CD1	2.48	0.48
9:D:175:LEU:HD23	9:D:182:ILE:HD13	1.93	0.48
20:O:32:SER:O	20:O:33:ASP:OD1	2.31	0.48
32:a:644:A:H2'	32:a:645:C:O4'	2.13	0.48
6:A:19:VAL:HB	32:a:2063:C:H1'	1.96	0.48
22:Q:3:THR:HG22	22:Q:66:THR:HG1	1.79	0.48
32:a:2327:A:H2'	32:a:2328:A:C8	2.47	0.48
7:B:918:A:H2'	7:B:919:A:O4'	2.14	0.48
14:I:108:LYS:HG2	14:I:121:LEU:HD11	1.96	0.48
28:W:226:THR:HG22	28:W:244:ILE:CD1	2.43	0.48
7:B:767:A:H2'	7:B:768:A:O4'	2.14	0.48
32:a:244:A:C2	32:a:255:A:C4	3.02	0.48
8:C:185:ALA:HB3	8:C:196:VAL:HG13	1.96	0.48
14:I:3:MET:HE1	14:I:9:ASP:HB2	1.95	0.48
16:K:7:ARG:HD2	16:K:73:LEU:HD11	1.95	0.48
29:X:23:A:H2'	29:X:24:G:C8	2.49	0.48
32:a:1433:A:H2'	32:a:1434:A:O4'	2.14	0.48
44:m:24:MET:HE1	44:m:40:LYS:HD3	1.95	0.48
48:q:3:ALA:HB2	48:q:101:ILE:HG21	1.96	0.48
49:r:95:ARG:HH21	49:r:97:LEU:HD21	1.79	0.48
10:E:101:VAL:HG12	10:E:105:MET:HE2	1.96	0.48
37:f:30:ARG:N	37:f:159:THR:HG1	2.12	0.48
8:C:217:VAL:O	8:C:221:VAL:HG23	2.14	0.48
13:H:69:VAL:O	13:H:138:ARG:HG3	2.14	0.48
14:I:102:ALA:HB3	14:I:113:ASP:HB3	1.96	0.48
18:M:74:LEU:HD23	18:M:104:CYS:SG	2.53	0.48
32:a:2063:C:O2	32:a:2450:A:N1	2.47	0.48
34:c:181:MET:HB3	34:c:268:VAL:HB	1.96	0.48
45:n:35:ILE:HG21	45:n:71:ALA:HA	1.95	0.48
7:B:371:A:H2'	7:B:372:C:O4'	2.14	0.47
7:B:716:A:N3	17:L:119:ASN:O	2.47	0.47
18:M:110:ARG:HB3	18:M:119:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1754:A:C8	46:o:94:LYS:HE2	2.50	0.47
39:h:12:LEU:HD22	39:h:19:VAL:HG11	1.95	0.47
42:k:129:LYS:HE3	42:k:129:LYS:HA	1.95	0.47
44:m:28:LEU:HD23	44:m:48:VAL:HG21	1.95	0.47
19:N:40:ALA:HB3	19:N:43:VAL:CG2	2.43	0.47
32:a:478:A:N1	32:a:500:G:H4'	2.30	0.47
32:a:2304:G:O2'	37:f:153:ASP:HB2	2.15	0.47
10:E:57:GLU:HG2	10:E:199:LEU:HD12	1.96	0.47
13:H:4:ARG:HG2	13:H:4:ARG:HH11	1.80	0.47
38:g:94:TYR:HA	38:g:106:SER:O	2.15	0.47
41:j:38:ILE:HD11	41:j:112:PHE:CZ	2.50	0.47
50:s:31:VAL:HG22	50:s:84:TYR:CD1	2.50	0.47
15:J:84:THR:CG2	15:J:98:LEU:HD13	2.41	0.47
32:a:1754:A:C8	46:o:94:LYS:CE	2.98	0.47
32:a:1853:A:N1	32:a:2087:G:H1'	2.29	0.47
37:f:100:PHE:CE1	37:f:104:ILE:HD11	2.49	0.47
7:B:627:G:H5'	22:Q:51:ARG:HH12	1.80	0.47
7:B:1391:U:H2'	7:B:1392:G:C8	2.50	0.47
12:G:29:ILE:HG21	12:G:64:VAL:CG1	2.45	0.47
32:a:120:U:H5''	32:a:122:G:OP2	2.14	0.47
32:a:263:G:H2'	32:a:264:C:O4'	2.14	0.47
32:a:2680:U:O2'	32:a:2681:C:H5'	2.15	0.47
34:c:203:ARG:HH21	34:c:203:ARG:HG3	1.79	0.47
40:i:84:ILE:HG23	40:i:84:ILE:O	2.14	0.47
14:I:18:GLN:CD	14:I:70:ALA:HB1	2.40	0.47
17:L:86:VAL:HG11	17:L:97:ILE:HD11	1.95	0.47
19:N:4:ILE:HD12	19:N:9:ILE:HD13	1.96	0.47
32:a:1296:G:OP1	32:a:2709:G:O2'	2.27	0.47
47:p:105:ALA:O	47:p:108:ALA:HB3	2.15	0.47
7:B:673:A:H2'	7:B:674:G:C8	2.50	0.47
8:C:63:ARG:O	8:C:64:LYS:C	2.58	0.47
41:j:98:ARG:C	41:j:99:ILE:HD12	2.40	0.47
5:4:34:LEU:N	5:4:34:LEU:HD23	2.29	0.47
7:B:152:A:N6	7:B:170:U:C2	2.83	0.47
15:J:21:ILE:HG12	15:J:63:LEU:HD23	1.96	0.47
17:L:30:THR:HG21	17:L:63:ALA:HB1	1.96	0.47
1:0:11:LEU:HD23	1:0:51:GLU:HA	1.96	0.46
7:B:1092:A:H5''	13:H:4:ARG:HH21	1.81	0.46
32:a:191:A:H2'	32:a:192:C:C6	2.50	0.46
53:v:59:LEU:HD12	53:v:80:ILE:HD12	1.97	0.46
7:B:390:U:H2'	7:B:391:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:166:ALA:HB3	8:C:191:SER:OG	2.15	0.46
9:D:153:VAL:HG12	9:D:157:LEU:HD21	1.98	0.46
13:H:97:ASN:HB3	13:H:101:MET:HE3	1.97	0.46
32:a:1028:A:N6	32:a:1125:G:H2'	2.31	0.46
32:a:2032:G:C8	35:d:150:MEQ:HE3	2.50	0.46
7:B:1251:A:H2'	7:B:1252:A:O4'	2.15	0.46
32:a:1637:A:H5'	32:a:1760:C:O2'	2.16	0.46
48:q:14:VAL:HG11	48:q:20:VAL:HG21	1.97	0.46
52:u:61:LEU:HD13	52:u:61:LEU:N	2.30	0.46
7:B:51:A:N7	7:B:114:U:O2'	2.46	0.46
9:D:42:TYR:CZ	9:D:90:VAL:HG11	2.50	0.46
9:D:111:LEU:CD1	9:D:146:ALA:HB2	2.43	0.46
12:G:22:ILE:HG23	12:G:39:LEU:HD11	1.98	0.46
32:a:742:A:H2'	32:a:743:A:C8	2.50	0.46
32:a:1720:U:H2'	32:a:1721:G:O4'	2.15	0.46
35:d:180:VAL:HG22	35:d:187:LEU:CD1	2.46	0.46
32:a:788:A:OP1	32:a:790:U:H5	1.99	0.46
32:a:928:A:C2	56:y:47:MET:HE1	2.50	0.46
34:c:144:VAL:HB	34:c:154:LEU:HB2	1.96	0.46
35:d:14:ILE:HD12	35:d:179:ARG:NH2	2.30	0.46
7:B:592:G:H2'	7:B:593:U:O4'	2.16	0.46
10:E:15:GLU:HG3	10:E:19:LEU:HD11	1.96	0.46
14:I:10:MET:HE1	14:I:36:ILE:CG2	2.45	0.46
36:e:175:ILE:HD11	36:e:199:MET:HE1	1.98	0.46
7:B:1304:G:C6	7:B:1305:G:N1	2.83	0.46
7:B:1476:A:H2'	7:B:1477:U:O4'	2.16	0.46
28:W:115:VAL:HB	28:W:162:ILE:CG2	2.46	0.46
32:a:1426:G:C6	32:a:1427:A:C6	3.03	0.46
42:k:19:LEU:CD2	42:k:27:LEU:HD13	2.45	0.46
10:E:154:ARG:HH11	10:E:154:ARG:CG	2.28	0.46
28:W:236:HIS:HB3	32:a:2602:A:H61	1.81	0.46
36:e:146:VAL:HA	36:e:185:LYS:O	2.16	0.46
45:n:106:LEU:HD23	45:n:106:LEU:C	2.41	0.46
8:C:200:ILE:N	8:C:200:ILE:HD12	2.30	0.46
15:J:44:ALA:O	15:J:48:VAL:HG23	2.16	0.46
29:X:75:C:H2'	29:X:76:A:O4'	2.15	0.46
35:d:121:THR:HB	35:d:127:PHE:CD2	2.51	0.46
23:R:25:ILE:HB	23:R:42:THR:HG23	1.96	0.46
32:a:476:G:H4'	32:a:502:A:N1	2.31	0.46
32:a:2026:U:H2'	32:a:2027:G:O4'	2.16	0.46
47:p:90:ILE:HG23	48:q:4:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:t:97:LYS:O	51:t:98:SER:CB	2.64	0.46
7:B:545:C:OP1	10:E:58:LYS:NZ	2.49	0.45
10:E:107:PHE:CG	10:E:145:ILE:HD11	2.50	0.45
19:N:71:ARG:NH2	37:f:113:ASP:OD2	2.49	0.45
28:W:100:LEU:O	28:W:101:LEU:C	2.59	0.45
32:a:1848:A:C8	32:a:1848:A:H5''	2.50	0.45
32:a:2237:G:O2'	32:a:2239:G:N7	2.47	0.45
41:j:9:ASN:OD1	41:j:18:ARG:NH1	2.48	0.45
45:n:35:ILE:HG23	45:n:74:VAL:HG21	1.97	0.45
52:u:77:VAL:HG23	52:u:89:ILE:HG12	1.97	0.45
7:B:718:A:C4	17:L:118:HIS:CD2	3.05	0.45
26:U:35:VAL:CG1	26:U:79:LEU:HD22	2.47	0.45
32:a:207:A:H2'	32:a:208:C:O4'	2.15	0.45
32:a:578:G:H21	32:a:1252:G:N2	2.14	0.45
32:a:1141:U:H4'	32:a:1142:A:O4'	2.16	0.45
33:b:24:G:N7	33:b:56:G:H2'	2.31	0.45
36:e:21:ARG:HD3	36:e:106:LYS:HB3	1.97	0.45
18:M:68:GLY:O	18:M:99:ARG:NH1	2.43	0.45
32:a:160:A:C6	32:a:161:A:C6	3.04	0.45
32:a:2233:U:H2'	32:a:2234:G:C8	2.52	0.45
32:a:1664:A:N3	41:j:67:LYS:NZ	2.65	0.45
47:p:97:ASP:OD1	48:q:13:ARG:NE	2.48	0.45
53:v:38:VAL:HG12	53:v:59:LEU:HB2	1.98	0.45
7:B:60:A:N1	7:B:107:G:O2'	2.42	0.45
7:B:381:C:H2'	7:B:382:A:O4'	2.16	0.45
7:B:663:A:H5'	7:B:836:G:OP1	2.17	0.45
7:B:868:C:H2'	7:B:869:G:O4'	2.17	0.45
32:a:84:A:N1	32:a:98:G:O2'	2.43	0.45
32:a:1332:G:N7	32:a:1609:A:O2'	2.48	0.45
32:a:1778:U:H2'	32:a:1784:A:N6	2.32	0.45
32:a:2352:A:C4	32:a:2366:A:C2	3.04	0.45
8:C:76:ALA:O	8:C:77:SER:C	2.59	0.45
8:C:210:VAL:HG12	8:C:214:LEU:CD1	2.45	0.45
9:D:35:SER:OG	9:D:59:ARG:NH2	2.49	0.45
11:F:75:ALA:HB1	11:F:149:SER:HB3	1.99	0.45
16:K:52:LEU:HD11	16:K:59:LYS:HD2	1.98	0.45
32:a:196:A:O2'	32:a:805:G:O6	2.29	0.45
32:a:701:G:C6	32:a:702:U:C5	3.05	0.45
32:a:2494:G:O2'	43:l:79:ALA:HA	2.17	0.45
40:i:110:PRO:O	40:i:115:GLY:HA3	2.17	0.45
7:B:66:A:C6	7:B:67:C:C5	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1144:G:H21	7:B:1146:A:H62	1.62	0.45
8:C:47:VAL:HB	8:C:48:PRO:CD	2.47	0.45
10:E:129:VAL:HG21	10:E:146:ARG:HH11	1.81	0.45
32:a:1739:A:H2'	32:a:1740:G:O4'	2.17	0.45
7:B:405:U:O4	10:E:2:ALA:N	2.50	0.45
7:B:993:G:H2'	7:B:993:G:N3	2.32	0.45
32:a:445:C:N4	32:a:446:G:C6	2.85	0.45
32:a:2748:A:C2	32:a:2757:A:C5	3.05	0.45
42:k:82:LEU:HD22	42:k:90:VAL:HG21	1.98	0.45
12:G:51:ILE:CG2	12:G:85:ILE:HD12	2.47	0.45
28:W:9:LEU:HA	28:W:12:LEU:HD23	1.99	0.45
32:a:1340:U:OP2	50:s:82:LYS:NZ	2.46	0.45
32:a:1424:G:H2'	32:a:1425:G:O4'	2.16	0.45
32:a:2014:A:H2'	32:a:2015:A:C8	2.52	0.45
35:d:25:THR:HG21	35:d:193:VAL:CG2	2.47	0.45
35:d:35:THR:HG22	35:d:73:VAL:HG21	1.98	0.45
36:e:138:LEU:HD22	36:e:143:LEU:CD1	2.46	0.45
51:t:35:ILE:HD13	51:t:64:ALA:HA	1.99	0.45
7:B:28:A:O2'	7:B:296:U:OP1	2.21	0.45
32:a:1266:G:O2'	32:a:2012:G:O6	2.30	0.45
34:c:70:ASN:O	34:c:72:ASP:N	2.50	0.45
37:f:29:PRO:HB2	37:f:169:LEU:HD22	1.99	0.45
12:G:88:MET:HG2	12:G:90:MET:HE2	2.00	0.44
18:M:40:THR:HG23	18:M:90:LEU:HD22	1.98	0.44
32:a:833:A:H2'	32:a:834:G:C8	2.52	0.44
36:e:105:LEU:HD23	36:e:105:LEU:HA	1.86	0.44
6:A:13:HIS:CG	32:a:2611:C:C6	3.06	0.44
7:B:690:G:H2'	7:B:691:G:O4'	2.17	0.44
12:G:4:TYR:CE1	12:G:91:ARG:HG2	2.52	0.44
35:d:168:GLU:O	35:d:170:VAL:HG23	2.16	0.44
39:h:37:VAL:HG22	39:h:38:PRO:HD2	1.98	0.44
44:m:55:ALA:HA	44:m:80:PHE:CE2	2.52	0.44
7:B:1332:A:C2	7:B:1333:A:C4	3.05	0.44
7:B:1456:A:H2'	7:B:1457:G:O4'	2.17	0.44
32:a:585:G:O6	32:a:1251:C:O2'	2.25	0.44
32:a:2392:A:C2	42:k:55:MET:HE3	2.53	0.44
45:n:7:ARG:NH1	45:n:95:SER:O	2.50	0.44
28:W:317:VAL:HG21	28:W:332:VAL:HG21	2.00	0.44
32:a:545:U:O2'	32:a:548:G:N2	2.50	0.44
4:3:2:LYS:NZ	32:a:2478:A:OP2	2.34	0.44
7:B:524:G:H2'	7:B:525:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:100:MET:CE	8:C:151:ILE:HD12	2.47	0.44
8:C:161:LEU:HD22	8:C:176:ALA:HB2	1.99	0.44
14:I:105:SER:HB2	14:I:126:ILE:HD11	1.99	0.44
17:L:61:PHE:O	17:L:64:GLN:HB3	2.18	0.44
22:Q:36:VAL:HG23	22:Q:36:VAL:O	2.15	0.44
26:U:54:MET:HE3	26:U:54:MET:HB3	1.92	0.44
32:a:578:G:OP1	32:a:1255:U:O2'	2.33	0.44
32:a:1996:C:OP1	41:j:31:ARG:NE	2.51	0.44
37:f:65:PRO:HB3	37:f:89:VAL:HG13	1.98	0.44
56:y:24:LEU:HD11	56:y:54:MET:CE	2.47	0.44
12:G:3:HIS:NE2	12:G:95:ALA:HB2	2.33	0.44
19:N:51:GLY:O	19:N:55:THR:HG23	2.16	0.44
32:a:1183:U:H2'	32:a:1184:U:C6	2.53	0.44
32:a:1378:A:O2'	32:a:1380:G:N7	2.50	0.44
32:a:2244:U:O2'	32:a:2245:U:H5'	2.18	0.44
32:a:2469:A:H4'	43:l:55:ARG:CD	2.47	0.44
33:b:29:A:H2'	33:b:30:C:O4'	2.18	0.44
14:I:7:ILE:HD11	14:I:32:LEU:HD23	1.99	0.44
19:N:89:LEU:O	19:N:93:ARG:HG2	2.17	0.44
32:a:223:A:N1	32:a:407:G:O2'	2.41	0.44
32:a:1313:U:O2	32:a:1313:U:C2'	2.66	0.44
40:i:114:LEU:HG	40:i:118:MET:HE3	2.00	0.44
10:E:130:VAL:HG11	10:E:135:TYR:CG	2.53	0.44
14:I:10:MET:HE1	14:I:36:ILE:HG21	2.00	0.44
32:a:585:G:N7	47:p:6:ARG:NH2	2.43	0.44
32:a:586:A:N1	32:a:809:G:O2'	2.50	0.44
32:a:1156:A:C8	47:p:51:ARG:HG2	2.53	0.44
32:a:1469:A:H2'	32:a:1470:A:C8	2.53	0.44
32:a:1618:6MZ:C9	32:a:1618:6MZ:N1	2.80	0.44
38:g:35:ARG:HG3	38:g:75:MET:SD	2.58	0.44
7:B:127:G:N2	23:R:63:GLU:OE1	2.43	0.44
28:W:162:ILE:HG23	28:W:162:ILE:O	2.18	0.44
32:a:58:G:O2'	32:a:73:A:N1	2.49	0.44
46:o:102:GLU:OE1	46:o:102:GLU:N	2.51	0.44
7:B:736:C:H2'	7:B:737:C:C6	2.53	0.43
11:F:156:LYS:HD3	14:I:71:VAL:HG13	2.00	0.43
31:Z:38:A:H3'	31:Z:39:U:H5''	2.00	0.43
32:a:1021:A:H3'	32:a:1021:A:N3	2.33	0.43
32:a:2520:C:C6	32:a:2567:G:H1'	2.52	0.43
41:j:1:MET:HE3	41:j:32:TYR:CZ	2.53	0.43
1:0:38:LYS:HB2	1:0:49:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:240:G:H4'	7:B:240:G:OP1	2.18	0.43
7:B:1305:G:N2	7:B:1331:G:H1'	2.33	0.43
8:C:187:VAL:HG21	8:C:199:VAL:HG13	1.99	0.43
12:G:42:TRP:CD2	12:G:102:MET:HG2	2.53	0.43
25:T:36:ARG:HH12	25:T:75:ALA:HB3	1.83	0.43
32:a:558:U:OP1	40:i:113:PRO:HD2	2.17	0.43
32:a:682:G:N2	32:a:796:C:C2	2.87	0.43
36:e:149:ILE:CD1	36:e:186:VAL:HG13	2.48	0.43
49:r:20:VAL:HG11	49:r:44:ALA:HA	2.00	0.43
10:E:105:MET:HE3	10:E:107:PHE:CE2	2.54	0.43
11:F:13:GLU:HG2	11:F:39:VAL:HG12	1.99	0.43
23:R:18:GLU:O	23:R:19:LYS:HB2	2.18	0.43
32:a:1731:G:C6	32:a:1733:G:C5	3.06	0.43
32:a:1820:U:OP1	34:c:177:ARG:NE	2.41	0.43
32:a:2013:A:H4'	49:r:96:ILE:HD13	1.99	0.43
46:o:31:TRP:CH2	46:o:40:LEU:HD11	2.53	0.43
7:B:495:A:C2	7:B:496:A:C6	3.06	0.43
7:B:1360:A:OP2	20:O:75:ARG:NH2	2.51	0.43
32:a:1204:A:H4'	32:a:1205:A:H5''	2.00	0.43
32:a:2800:A:C2	32:a:2895:G:H1'	2.53	0.43
17:L:97:ILE:HG22	27:V:12:PHE:HZ	1.82	0.43
22:Q:59:HIS:O	22:Q:63:GLN:HG2	2.18	0.43
28:W:322:ILE:O	28:W:323:ASN:C	2.61	0.43
32:a:1750:G:O2'	32:a:2860:A:N1	2.47	0.43
7:B:499:A:N1	7:B:546:A:O2'	2.47	0.43
8:C:184:PHE:CE2	8:C:198:PHE:CD1	3.06	0.43
15:J:7:TYR:CG	15:J:8:GLY:N	2.86	0.43
28:W:151:ALA:HB2	28:W:162:ILE:HD12	2.00	0.43
28:W:245:ARG:HG3	28:W:256:GLU:HG2	2.00	0.43
32:a:265:A:N1	32:a:427:U:O2'	2.51	0.43
32:a:2223:G:H8	32:a:2223:G:H5''	1.83	0.43
36:e:175:ILE:HD11	36:e:199:MET:CE	2.49	0.43
3:2:64:TYR:CE2	32:a:242:G:H5''	2.53	0.43
7:B:243:A:C2	7:B:246:A:C8	3.06	0.43
14:I:11:LEU:HD22	14:I:75:ILE:CD1	2.43	0.43
15:J:18:ARG:NH1	15:J:66:THR:OG1	2.45	0.43
20:O:93:ILE:HG21	20:O:96:LEU:HD22	2.01	0.43
32:a:479:A:N3	32:a:481:G:H5''	2.34	0.43
32:a:2066:C:O2'	32:a:2067:G:H5'	2.18	0.43
38:g:38:ASN:C	38:g:40:ALA:H	2.26	0.43
47:p:58:ARG:HA	47:p:61:TRP:CE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:w:7:VAL:CG2	54:w:51:VAL:HG23	2.49	0.43
10:E:95:GLU:HA	10:E:100:ASN:ND2	2.34	0.43
10:E:125:VAL:HG11	10:E:135:TYR:HE2	1.83	0.43
13:H:103:TRP:CG	13:H:137:LYS:HD3	2.53	0.43
14:I:78:VAL:HG21	14:I:128:TYR:CE1	2.54	0.43
49:r:59:GLU:OE1	49:r:66:ILE:HB	2.19	0.43
7:B:950:U:H2'	7:B:951:G:C8	2.54	0.43
32:a:542:C:H2'	32:a:543:G:C8	2.54	0.43
32:a:2431:U:O2'	32:a:2433:A:N7	2.49	0.43
33:b:73:A:C4	33:b:104:A:C2	3.07	0.43
7:B:1092:A:C5'	13:H:4:ARG:HH21	2.31	0.43
16:K:10:LEU:CB	16:K:18:ILE:HD11	2.49	0.43
16:K:57:VAL:HG23	16:K:58:ASN:N	2.34	0.43
28:W:137:ARG:HB3	28:W:137:ARG:NH1	2.34	0.43
32:a:2547:A:C2	32:a:2562:U:C2	3.07	0.43
8:C:91:PHE:CE1	8:C:150:GLY:HA2	2.54	0.42
28:W:248:HIS:HB2	28:W:274:LEU:HD11	1.99	0.42
32:a:1348:C:C5	32:a:1349:C:C5	3.07	0.42
28:W:261:ARG:NH2	29:X:74:C:O3'	2.51	0.42
32:a:1548:A:H2'	32:a:1549:A:C8	2.54	0.42
7:B:1297:G:H21	13:H:114:LYS:HB3	1.85	0.42
11:F:81:LEU:CD2	11:F:120:VAL:HG11	2.49	0.42
28:W:210:PRO:O	28:W:211:ASP:C	2.62	0.42
32:a:1746:A:H2'	32:a:1747:U:C6	2.54	0.42
32:a:2028:U:C4	32:a:2029:G:C6	3.07	0.42
5:4:12:ILE:HD13	5:4:28:VAL:CG1	2.49	0.42
7:B:156:C:H2'	7:B:157:U:O4'	2.20	0.42
7:B:1086:U:H3	7:B:1099:G:H22	1.67	0.42
7:B:1303:C:N4	7:B:1304:G:C6	2.87	0.42
24:S:65:LEU:O	24:S:66:SER:C	2.63	0.42
26:U:54:MET:HE2	26:U:79:LEU:CD1	2.49	0.42
38:g:83:PHE:CE2	38:g:138:LYS:HB2	2.55	0.42
41:j:38:ILE:HD11	41:j:112:PHE:HZ	1.84	0.42
54:w:43:GLU:OE2	54:w:45:ARG:NH2	2.51	0.42
32:a:1042:G:C6	32:a:1043:C:C4	3.07	0.42
43:l:17:ASN:O	43:l:38:ARG:HD3	2.19	0.42
49:r:7:HIS:HB2	49:r:50:VAL:HG22	2.01	0.42
56:y:41:THR:HG22	56:y:43:ALA:H	1.83	0.42
7:B:555:U:H2'	7:B:556:C:C6	2.55	0.42
7:B:1058:G:H2'	7:B:1059:C:O4'	2.19	0.42
18:M:47:SER:O	18:M:48:ALA:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1450:G:C6	32:a:1451:C:N4	2.88	0.42
32:a:1678:A:H2'	32:a:1679:A:O4'	2.19	0.42
32:a:2291:U:H2'	32:a:2292:U:C6	2.54	0.42
32:a:2715:C:C4	32:a:2716:C:C5	3.07	0.42
42:k:77:ILE:HD11	42:k:101:ILE:HG21	2.00	0.42
3:2:45:ARG:N	3:2:46:PRO:HD2	2.34	0.42
7:B:244:U:O4	7:B:906:A:H1'	2.20	0.42
8:C:167:ASP:CG	8:C:191:SER:HA	2.45	0.42
26:U:28:MET:HE1	26:U:67:ILE:CG2	2.49	0.42
32:a:948:C:H1'	32:a:984:A:C8	2.55	0.42
32:a:1601:G:OP1	50:s:64:LYS:NZ	2.49	0.42
32:a:2563:U:H1'	32:a:2566:A:C6	2.55	0.42
39:h:26:ALA:O	39:h:31:VAL:HG23	2.20	0.42
7:B:409:U:P	10:E:23:SER:HG	2.43	0.42
7:B:867:G:O2'	7:B:873:A:N1	2.52	0.42
8:C:151:ILE:HG22	8:C:151:ILE:O	2.20	0.42
9:D:116:VAL:O	9:D:119:SER:HB3	2.20	0.42
17:L:31:ILE:HG12	17:L:46:THR:HG22	2.02	0.42
32:a:83:A:OP1	51:t:2:ALA:HB2	2.20	0.42
32:a:460:A:H2'	32:a:461:C:O4'	2.20	0.42
32:a:2251:OMG:HM23	32:a:2251:OMG:H1'	1.84	0.42
32:a:2618:G:H21	35:d:155:VAL:HG21	1.84	0.42
7:B:744:C:H2'	7:B:745:G:C8	2.54	0.42
7:B:921:U:H2'	7:B:922:G:O4'	2.19	0.42
12:G:2:ARG:HB3	12:G:91:ARG:HH11	1.85	0.42
12:G:90:MET:HE3	12:G:90:MET:HB2	1.87	0.42
14:I:25:VAL:HG13	14:I:63:LEU:HD11	2.02	0.42
35:d:146:ILE:HA	35:d:159:LYS:HE3	2.02	0.42
43:l:12:MET:HE3	43:l:12:MET:HB2	1.82	0.42
45:n:26:LEU:HD23	45:n:92:PHE:HD1	1.85	0.42
7:B:413:G:O2'	7:B:428:G:N2	2.52	0.42
7:B:874:G:C6	7:B:875:U:C4	3.08	0.42
7:B:1152:A:OP1	16:K:70:HIS:ND1	2.48	0.42
23:R:27:ARG:NH1	23:R:29:VAL:HG21	2.35	0.42
28:W:21:ALA:HB3	28:W:22:LEU:HD22	2.02	0.42
28:W:126:LEU:HD21	28:W:156:HIS:O	2.20	0.42
32:a:729:G:C5	34:c:207:LYS:HB2	2.55	0.42
32:a:743:A:OP1	35:d:135:GLY:HA2	2.20	0.42
32:a:2564:A:C2	32:a:2647:U:H4'	2.55	0.42
36:e:5:LEU:N	36:e:5:LEU:HD12	2.34	0.42
7:B:511:C:C2	7:B:512:U:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:575:G:O2'	7:B:821:G:OP2	2.34	0.41
7:B:1376:U:OP2	13:H:25:LYS:NZ	2.45	0.41
32:a:431:U:O5'	32:a:431:U:H6	2.03	0.41
37:f:96:MET:CE	37:f:97:TRP:CE2	3.03	0.41
7:B:109:A:C6	7:B:326:G:C6	3.08	0.41
7:B:1179:A:H5''	15:J:104:VAL:HG12	2.01	0.41
32:a:26:G:H1'	32:a:514:A:N6	2.35	0.41
32:a:554:U:O4	32:a:555:G:C6	2.73	0.41
32:a:918:A:H5''	33:b:97:C:O2'	2.20	0.41
32:a:2521:C:C2	32:a:2545:G:N2	2.89	0.41
32:a:2639:A:H2'	32:a:2640:G:O4'	2.20	0.41
7:B:6:G:N2	11:F:103:THR:HG23	2.35	0.41
7:B:1349:A:C2	7:B:1374:A:C4	3.08	0.41
7:B:1477:U:H2'	7:B:1478:U:C6	2.56	0.41
9:D:14:ILE:HD12	9:D:14:ILE:N	2.35	0.41
15:J:88:MET:HE1	15:J:104:VAL:HG13	2.02	0.41
15:J:118:LEU:HD22	15:J:124:ARG:HG2	2.02	0.41
19:N:83:LEU:HD23	19:N:83:LEU:HA	1.95	0.41
28:W:180:GLY:HA3	28:W:307:ASN:ND2	2.36	0.41
32:a:580:U:O3'	47:p:31:VAL:HG13	2.20	0.41
32:a:659:G:O2'	36:e:95:LYS:O	2.33	0.41
32:a:667:U:H2'	32:a:668:A:O4'	2.21	0.41
48:q:74:ILE:N	48:q:74:ILE:HD12	2.35	0.41
5:4:24:ILE:HD13	37:f:106:ILE:HD12	2.03	0.41
7:B:374:A:C6	7:B:375:U:C4	3.08	0.41
7:B:901:A:O2'	7:B:1513:A:OP1	2.30	0.41
8:C:97:LEU:HB2	8:C:100:MET:HG3	2.03	0.41
12:G:88:MET:HE1	24:S:61:ARG:HG2	2.01	0.41
32:a:537:G:H5''	40:i:5:THR:HG21	2.02	0.41
32:a:1007:C:OP1	40:i:37:ARG:NH2	2.52	0.41
32:a:1367:A:C5	32:a:1368:G:H1'	2.55	0.41
41:j:99:ILE:HD13	41:j:118:LEU:CB	2.50	0.41
45:n:74:VAL:O	45:n:78:VAL:HG12	2.20	0.41
7:B:116:A:H8	7:B:116:A:O5'	2.03	0.41
12:G:4:TYR:CD2	12:G:71:ILE:HG13	2.56	0.41
26:U:31:PHE:CD2	26:U:57:ILE:HD13	2.56	0.41
32:a:157:C:H2'	32:a:158:U:O4'	2.21	0.41
32:a:703:U:H2'	32:a:704:G:O4'	2.20	0.41
34:c:107:PRO:HD2	34:c:110:LEU:HD22	2.01	0.41
38:g:24:ILE:HD12	38:g:37:LEU:CD2	2.50	0.41
39:h:3:VAL:O	39:h:18:GLN:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:74:ILE:HG23	50:s:74:ILE:O	2.20	0.41
7:B:1128:C:O2'	7:B:1147:C:N3	2.51	0.41
28:W:245:ARG:NH2	32:a:2556:C:O2	2.53	0.41
32:a:563:A:C4	32:a:2018:G:C2	3.08	0.41
32:a:756:A:H2'	32:a:757:G:O4'	2.19	0.41
32:a:1039:A:H2'	32:a:1040:A:O4'	2.20	0.41
32:a:1234:U:O4	32:a:1235:G:C6	2.74	0.41
32:a:1681:G:N3	32:a:1762:A:H2'	2.36	0.41
32:a:1744:A:H3'	32:a:1745:A:H8	1.86	0.41
7:B:604:G:C2	7:B:635:A:C2	3.09	0.41
7:B:1463:U:H2'	7:B:1464:U:C6	2.56	0.41
8:C:165:ASP:OD1	8:C:204:ASP:OD2	2.37	0.41
10:E:202:GLU:CD	11:F:112:ARG:HH12	2.28	0.41
12:G:18:VAL:HG21	12:G:58:HIS:CE1	2.56	0.41
20:O:10:GLU:HG3	20:O:63:ARG:HD2	2.01	0.41
28:W:236:HIS:HB3	32:a:2602:A:N6	2.35	0.41
32:a:749:A:H4'	32:a:1271:G:N3	2.36	0.41
32:a:956:G:O6	43:l:14:LYS:HE3	2.19	0.41
32:a:1263:U:O2'	57:z:8:PRO:HD2	2.20	0.41
32:a:1417:C:C4'	32:a:1587:G:H21	2.34	0.41
32:a:1676:A:H2'	32:a:1677:A:O4'	2.20	0.41
32:a:1877:A:H2'	32:a:1878:G:O4'	2.21	0.41
32:a:2094:A:H5''	39:h:25:TYR:CD2	2.56	0.41
32:a:2273:A:H2'	32:a:2274:A:C8	2.56	0.41
32:a:2328:A:H2'	32:a:2329:U:C6	2.55	0.41
32:a:2788:C:H2'	32:a:2789:C:C6	2.56	0.41
34:c:29:PRO:CG	34:c:34:LEU:HD11	2.47	0.41
7:B:580:C:H2'	7:B:581:G:O4'	2.20	0.41
7:B:1516:2MG:HM21	7:B:1519:A:N7	2.35	0.41
11:F:133:PRO:O	11:F:137:VAL:HG23	2.20	0.41
12:G:51:ILE:HG21	12:G:85:ILE:HD12	2.03	0.41
17:L:67:ALA:HB2	17:L:96:THR:HG23	2.01	0.41
28:W:178:GLU:OE1	28:W:308:ARG:NH1	2.52	0.41
32:a:685:A:H5''	32:a:788:A:H62	1.85	0.41
32:a:1792:G:O2'	32:a:1830:C:OP1	2.37	0.41
34:c:76:ALA:HB2	34:c:96:TYR:CE1	2.55	0.41
35:d:2:ILE:HG23	35:d:88:GLU:OE1	2.21	0.41
36:e:179:SER:O	36:e:183:PHE:HD2	2.03	0.41
40:i:4:PHE:O	47:p:64:ARG:NH2	2.46	0.41
40:i:111:LYS:NZ	62:i:201:HOH:O	2.48	0.41
47:p:61:TRP:CZ2	47:p:93:LYS:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:x:46:VAL:O	55:x:50:VAL:HG23	2.20	0.41
6:A:17:ILE:CG2	6:A:19:VAL:HG13	2.50	0.41
6:A:19:VAL:HG12	32:a:2062:A:H2	1.86	0.41
7:B:323:U:H2'	7:B:324:G:O4'	2.20	0.41
11:F:56:VAL:N	11:F:57:PRO:CD	2.84	0.41
15:J:30:ILE:HA	15:J:65:ILE:O	2.21	0.41
23:R:75:LEU:C	23:R:75:LEU:HD13	2.46	0.41
28:W:308:ARG:HD3	28:W:340:LEU:HD13	2.01	0.41
32:a:373:U:O2'	32:a:423:A:H1'	2.20	0.41
32:a:871:U:H5''	43:l:68:PHE:CZ	2.56	0.41
32:a:1003:G:O2'	32:a:1010:A:N1	2.50	0.41
32:a:1024:G:C6	32:a:1025:G:C6	3.09	0.41
32:a:1148:U:H2'	32:a:1149:G:O4'	2.21	0.41
32:a:2250:G:OP2	32:a:2275:C:H2'	2.21	0.41
32:a:2812:G:H2'	32:a:2813:A:O4'	2.21	0.41
34:c:144:VAL:HG12	34:c:145:GLU:O	2.21	0.41
39:h:31:VAL:HB	39:h:32:PRO:HD3	2.02	0.41
44:m:51:LEU:HD12	44:m:51:LEU:HA	1.93	0.41
46:o:18:PRO:HG3	46:o:84:ILE:O	2.21	0.41
7:B:266:G:N3	7:B:266:G:H2'	2.35	0.41
8:C:54:LEU:CD2	8:C:217:VAL:HG12	2.51	0.41
8:C:199:VAL:C	8:C:200:ILE:HD12	2.46	0.41
15:J:35:LEU:HD23	15:J:49:ARG:NH1	2.36	0.41
17:L:84:VAL:CG2	17:L:107:ILE:HD12	2.51	0.41
28:W:342:GLU:HB2	28:W:343:PRO:HD3	2.02	0.41
32:a:247:G:H4'	32:a:386:G:C5	2.56	0.41
32:a:395:U:O2'	32:a:396:G:N7	2.50	0.41
32:a:2544:G:H2'	32:a:2545:G:O4'	2.20	0.41
3:2:27:ALA:O	3:2:28:ASN:HB2	2.22	0.40
10:E:105:MET:HG3	10:E:171:LEU:HD21	2.03	0.40
18:M:28:PRO:HB2	18:M:29:GLN:NE2	2.37	0.40
28:W:191:GLU:OE1	28:W:194:GLY:N	2.54	0.40
32:a:563:A:H1'	32:a:2018:G:N2	2.36	0.40
32:a:571:U:C4	32:a:2030:A:C6	3.09	0.40
32:a:2573:C:O2	32:a:2573:C:H2'	2.21	0.40
32:a:2687:U:H2'	32:a:2688:G:O4'	2.21	0.40
42:k:132:ARG:HG3	42:k:142:ILE:HD12	2.03	0.40
7:B:202:G:H1	7:B:215:C:H42	1.69	0.40
7:B:251:G:C6	7:B:266:G:C6	3.10	0.40
7:B:1062:U:H2'	7:B:1063:C:C6	2.56	0.40
8:C:186:ILE:HD13	8:C:200:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:115:LEU:HB3	11:F:120:VAL:CG2	2.51	0.40
32:a:637:A:OP1	42:k:130:GLY:HA3	2.22	0.40
32:a:1115:G:O2'	32:a:1116:G:O5'	2.29	0.40
32:a:1562:U:H2'	32:a:1563:U:O4'	2.21	0.40
33:b:104:A:H2'	33:b:105:G:O4'	2.20	0.40
36:e:48:THR:HG23	36:e:88:ARG:HH12	1.86	0.40
54:w:7:VAL:HG23	54:w:51:VAL:HG23	2.03	0.40
57:z:40:ARG:HH11	57:z:40:ARG:HG3	1.87	0.40
7:B:1226:C:H4'	25:T:80:TYR:CZ	2.56	0.40
32:a:627:A:C6	32:a:637:A:C8	3.09	0.40
32:a:700:G:O2'	32:a:1632:A:N3	2.48	0.40
32:a:910:A:N3	32:a:2264:C:O2'	2.53	0.40
34:c:78:VAL:HG21	34:c:110:LEU:HD21	2.02	0.40
55:x:14:LEU:HD12	55:x:14:LEU:HA	1.92	0.40
7:B:235:C:H2'	7:B:236:A:C8	2.56	0.40
7:B:598:U:H4'	14:I:86:TYR:CG	2.57	0.40
7:B:928:G:O2'	7:B:1533:C:OP1	2.39	0.40
7:B:1237:C:C2'	7:B:1238:A:OP1	2.70	0.40
32:a:825:A:H2'	32:a:826:U:O4'	2.22	0.40
32:a:2564:A:C6	32:a:2565:A:N1	2.89	0.40
32:a:2849:U:H4'	32:a:2868:A:C2	2.57	0.40
42:k:82:LEU:HB3	42:k:120:VAL:HG11	2.03	0.40
45:n:70:ALA:O	45:n:74:VAL:HG23	2.22	0.40
47:p:91:ASP:C	47:p:91:ASP:OD1	2.65	0.40
49:r:6:LYS:HA	49:r:103:ILE:O	2.21	0.40
7:B:421:U:O2	7:B:421:U:O4'	2.38	0.40
7:B:527:G7M:O2'	7:B:535:A:N1	2.49	0.40
7:B:815:A:N7	7:B:1509:C:O2'	2.53	0.40
11:F:104:GLY:O	11:F:122:ASN:HA	2.22	0.40
18:M:85:GLY:O	18:M:96:HIS:ND1	2.52	0.40
22:Q:61:VAL:HG21	22:Q:67:ILE:HD11	2.04	0.40
32:a:1652:A:N6	44:m:11:ASN:OD1	2.47	0.40
34:c:136:PRO:O	34:c:139:SER:OG	2.36	0.40
45:n:35:ILE:HG12	45:n:106:LEU:HD12	2.04	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%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	7	7
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
5	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
6	A	17/19 (90%)	17 (100%)	0	0	100	100
8	C	222/241 (92%)	203 (91%)	17 (8%)	2 (1%)	14	17
9	D	204/233 (88%)	174 (85%)	30 (15%)	0	100	100
10	E	203/206 (98%)	191 (94%)	10 (5%)	2 (1%)	12	15
11	F	154/167 (92%)	143 (93%)	11 (7%)	0	100	100
12	G	101/135 (75%)	96 (95%)	2 (2%)	3 (3%)	3	2
13	H	151/179 (84%)	125 (83%)	23 (15%)	3 (2%)	6	5
14	I	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
15	J	125/130 (96%)	112 (90%)	10 (8%)	3 (2%)	4	4
16	K	96/103 (93%)	86 (90%)	7 (7%)	3 (3%)	3	2
17	L	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	7	7
18	M	121/124 (98%)	115 (95%)	4 (3%)	2 (2%)	7	7
19	N	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
20	O	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	12	15
21	P	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
22	Q	79/82 (96%)	73 (92%)	5 (6%)	1 (1%)	9	10
23	R	77/84 (92%)	72 (94%)	4 (5%)	1 (1%)	9	10
24	S	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
25	T	82/92 (89%)	77 (94%)	5 (6%)	0	100	100
26	U	84/87 (97%)	83 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	V	68/71 (96%)	65 (96%)	2 (3%)	1 (2%)	8	8
28	W	352/360 (98%)	327 (93%)	15 (4%)	10 (3%)	4	2
34	c	269/273 (98%)	254 (94%)	14 (5%)	1 (0%)	30	38
35	d	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
36	e	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	24	31
37	f	175/179 (98%)	163 (93%)	11 (6%)	1 (1%)	21	27
38	g	174/177 (98%)	160 (92%)	13 (8%)	1 (1%)	21	27
39	h	39/149 (26%)	33 (85%)	6 (15%)	0	100	100
40	i	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
41	j	121/123 (98%)	113 (93%)	7 (6%)	1 (1%)	16	20
42	k	142/144 (99%)	132 (93%)	9 (6%)	1 (1%)	18	23
43	l	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
44	m	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
45	n	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	14	17
46	o	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
47	p	115/118 (98%)	115 (100%)	0	0	100	100
48	q	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
49	r	108/110 (98%)	103 (95%)	4 (4%)	1 (1%)	14	17
50	s	91/100 (91%)	86 (94%)	4 (4%)	1 (1%)	11	13
51	t	100/104 (96%)	89 (89%)	6 (6%)	5 (5%)	1	1
52	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
53	v	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
54	w	75/78 (96%)	67 (89%)	8 (11%)	0	100	100
55	x	60/63 (95%)	55 (92%)	3 (5%)	2 (3%)	3	2
56	y	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	6	6
57	z	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
All	All	5855/6292 (93%)	5455 (93%)	348 (6%)	52 (1%)	16	17

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	H	5	ARG
13	H	130	ASN

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Mol	Chain	Res	Type
28	W	70	ASP
28	W	211	ASP
28	W	323	ASN
34	c	71	LYS
49	r	12	SER
51	t	98	SER
8	C	64	LYS
8	C	77	SER
12	G	33	GLU
13	H	113	ASP
16	K	31	ARG
16	K	57	VAL
27	V	65	ALA
28	W	143	ARG
28	W	212	ALA
50	s	89	GLU
51	t	39	ILE
51	t	97	LYS
51	t	99	ASN
55	x	37	LEU
56	y	4	THR
17	L	89	PRO
17	L	119	ASN
18	M	17	ALA
23	R	50	ASN
55	x	36	GLN
3	2	28	ASN
10	E	166	GLU
12	G	38	ARG
12	G	68	GLN
16	K	91	ASP
18	M	48	ALA
28	W	38	LEU
28	W	73	GLU
42	k	29	LYS
45	n	99	TYR
51	t	76	ALA
15	J	13	LYS
15	J	109	ARG
20	O	33	ASP
15	J	107	ASP
22	Q	80	LYS

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Mol	Chain	Res	Type
28	W	141	ALA
36	e	142	ALA
28	W	210	PRO
28	W	342	GLU
37	f	109	PRO
10	E	64	ILE
38	g	12	PRO
41	j	48	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	45 (98%)	1 (2%)	45	65
2	1	38/38 (100%)	37 (97%)	1 (3%)	40	59
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	55
5	4	55/62 (89%)	54 (98%)	1 (2%)	51	70
6	A	18/18 (100%)	17 (94%)	1 (6%)	19	28
8	C	186/199 (94%)	182 (98%)	4 (2%)	45	65
9	D	170/190 (90%)	163 (96%)	7 (4%)	27	41
10	E	172/173 (99%)	162 (94%)	10 (6%)	18	26
11	F	119/126 (94%)	118 (99%)	1 (1%)	73	86
12	G	90/116 (78%)	85 (94%)	5 (6%)	19	28
13	H	126/147 (86%)	125 (99%)	1 (1%)	73	86
14	I	104/105 (99%)	102 (98%)	2 (2%)	50	69
15	J	105/107 (98%)	102 (97%)	3 (3%)	37	55
16	K	86/90 (96%)	81 (94%)	5 (6%)	18	26
17	L	90/99 (91%)	89 (99%)	1 (1%)	65	81
18	M	103/104 (99%)	101 (98%)	2 (2%)	50	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	N	93/96 (97%)	91 (98%)	2 (2%)	45	65
20	O	83/84 (99%)	82 (99%)	1 (1%)	63	79
21	P	76/77 (99%)	76 (100%)	0	100	100
22	Q	65/65 (100%)	63 (97%)	2 (3%)	35	52
23	R	73/78 (94%)	72 (99%)	1 (1%)	59	76
24	S	57/65 (88%)	56 (98%)	1 (2%)	51	70
25	T	72/79 (91%)	70 (97%)	2 (3%)	38	56
26	U	65/66 (98%)	64 (98%)	1 (2%)	57	75
27	V	60/61 (98%)	59 (98%)	1 (2%)	53	72
28	W	294/300 (98%)	283 (96%)	11 (4%)	30	45
34	c	216/218 (99%)	213 (99%)	3 (1%)	59	76
35	d	163/163 (100%)	161 (99%)	2 (1%)	63	79
36	e	165/165 (100%)	162 (98%)	3 (2%)	51	70
37	f	148/150 (99%)	147 (99%)	1 (1%)	76	87
38	g	137/138 (99%)	132 (96%)	5 (4%)	31	47
39	h	32/114 (28%)	30 (94%)	2 (6%)	16	23
40	i	116/116 (100%)	115 (99%)	1 (1%)	70	84
41	j	104/104 (100%)	101 (97%)	3 (3%)	37	55
42	k	103/103 (100%)	101 (98%)	2 (2%)	50	69
43	l	109/109 (100%)	105 (96%)	4 (4%)	30	45
44	m	98/103 (95%)	96 (98%)	2 (2%)	48	67
45	n	86/87 (99%)	85 (99%)	1 (1%)	63	79
46	o	99/100 (99%)	99 (100%)	0	100	100
47	p	89/90 (99%)	88 (99%)	1 (1%)	65	81
48	q	84/84 (100%)	84 (100%)	0	100	100
49	r	93/93 (100%)	91 (98%)	2 (2%)	45	65
50	s	80/84 (95%)	78 (98%)	2 (2%)	42	60
51	t	83/85 (98%)	82 (99%)	1 (1%)	63	79
52	u	78/78 (100%)	76 (97%)	2 (3%)	40	59
53	v	58/63 (92%)	58 (100%)	0	100	100
54	w	67/68 (98%)	66 (98%)	1 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	x	54/55 (98%)	53 (98%)	1 (2%)	50	69
56	y	48/49 (98%)	48 (100%)	0	100	100
57	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4888/5147 (95%)	4781 (98%)	107 (2%)	45	65

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	27	LYS
2	1	1	MET
4	3	2	LYS
5	4	34	LEU
6	A	19	VAL
8	C	32	PHE
8	C	93	ASN
8	C	105	LYS
8	C	222	ARG
9	D	46	GLU
9	D	68	ILE
9	D	105	GLU
9	D	123	GLN
9	D	178	LEU
9	D	195	VAL
9	D	202	ILE
10	E	8	LYS
10	E	34	ILE
10	E	45	LYS
10	E	57	GLU
10	E	60	LYS
10	E	123	ILE
10	E	142	VAL
10	E	177	LYS
10	E	181	THR
10	E	188	ARG
11	F	162	GLU
12	G	17	GLN
12	G	37	HIS
12	G	74	LEU
12	G	91	ARG
12	G	102	MET
13	H	67	GLU

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Mol	Chain	Res	Type
14	I	56	LYS
14	I	107	SER
15	J	27	LYS
15	J	56	ASP
15	J	85	ARG
16	K	17	LEU
16	K	18	ILE
16	K	27	GLU
16	K	75	ASP
16	K	90	LEU
17	L	129	VAL
18	M	34	CYS
18	M	44	LYS
19	N	11	ASP
19	N	68	ASP
20	O	33	ASP
22	Q	12	LYS
22	Q	76	LYS
23	R	67	LEU
24	S	16	GLU
25	T	15	LEU
25	T	55	ARG
26	U	85	LYS
27	V	3	VAL
28	W	69	LEU
28	W	96	LEU
28	W	101	LEU
28	W	103	LYS
28	W	143	ARG
28	W	146	VAL
28	W	149	MET
28	W	254	VAL
28	W	255	VAL
28	W	271	LEU
28	W	356	LEU
34	c	4	VAL
34	c	132	MET
34	c	165	VAL
35	d	1	MET
35	d	12	THR
36	e	143	LEU
36	e	153	LEU

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Mol	Chain	Res	Type
36	e	191	ASP
37	f	120	LYS
38	g	15	VAL
38	g	34	THR
38	g	36	THR
38	g	72	LEU
38	g	86	LYS
39	h	6	LEU
39	h	9	VAL
40	i	17	VAL
41	j	58	LEU
41	j	76	VAL
41	j	93	GLN
42	k	112	LEU
42	k	129	LYS
43	l	36	VAL
43	l	53	MET
43	l	80	VAL
43	l	82	MET
44	m	51	LEU
44	m	98	LEU
45	n	35	ILE
47	p	112	LYS
49	r	62	ASP
49	r	66	ILE
50	s	89	GLU
50	s	93	LEU
51	t	52	LEU
52	u	61	LEU
52	u	62	THR
54	w	40	VAL
55	x	56	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	61	ASN
8	C	177	ASN
10	E	40	GLN
11	F	61	GLN
11	F	70	ASN
11	F	97	GLN

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Mol	Chain	Res	Type
13	H	68	ASN
15	J	110	GLN
17	L	118	HIS
19	N	14	HIS
21	P	40	GLN
21	P	62	GLN
23	R	9	GLN
23	R	51	ASN
26	U	3	ASN
26	U	82	GLN
28	W	97	GLN
28	W	307	ASN
28	W	349	GLN
34	c	86	ASN
36	e	9	GLN
36	e	90	GLN
36	e	92	HIS
37	f	37	ASN
38	g	30	ASN
38	g	73	ASN
38	g	88	GLN
38	g	116	GLN
39	h	20	ASN
40	i	76	HIS
41	j	93	GLN
43	l	60	GLN
43	l	97	GLN
45	n	98	GLN
45	n	100	HIS
46	o	52	ASN
47	p	20	GLN
47	p	81	ASN
48	q	6	GLN
48	q	43	ASN
49	r	9	HIS
49	r	40	ASN
50	s	48	GLN
51	t	27	ASN
51	t	54	GLN
51	t	74	ASN
52	u	49	ASN
53	v	57	HIS

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Mol	Chain	Res	Type
54	w	20	HIS
55	x	25	GLN
55	x	58	ASN
56	y	9	GLN
57	z	6	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	75/76 (98%)	18 (24%)	4 (5%)
30	Y	8/9 (88%)	0	0
31	Z	75/76 (98%)	41 (54%)	3 (4%)
32	a	2749/2903 (94%)	348 (12%)	0
33	b	118/120 (98%)	13 (11%)	0
7	B	1517/1534 (98%)	243 (16%)	24 (1%)
All	All	4542/4718 (96%)	663 (14%)	31 (0%)

All (663) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	B	4	U
7	B	5	U
7	B	6	G
7	B	7	A
7	B	8	A
7	B	9	G
7	B	22	G
7	B	32	A
7	B	39	G
7	B	44	A
7	B	47	C
7	B	48	C
7	B	50	A
7	B	51	A
7	B	58	C
7	B	65	A
7	B	66	A
7	B	70	U
7	B	71	A
7	B	72	A
7	B	75	G

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Mol	Chain	Res	Type
7	B	78	A
7	B	81	A
7	B	83	C
7	B	85	U
7	B	86	G
7	B	87	C
7	B	88	U
7	B	96	U
7	B	119	A
7	B	120	A
7	B	121	U
7	B	122	G
7	B	131	A
7	B	142	G
7	B	143	A
7	B	144	G
7	B	159	G
7	B	163	C
7	B	164	G
7	B	182	A
7	B	189	A
7	B	191	G
7	B	197	A
7	B	199	A
7	B	203	G
7	B	204	G
7	B	215	C
7	B	226	G
7	B	240	G
7	B	245	U
7	B	247	G
7	B	251	G
7	B	266	G
7	B	267	C
7	B	271	C
7	B	280	C
7	B	289	G
7	B	299	G
7	B	319	G
7	B	321	A
7	B	328	C
7	B	329	A

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Mol	Chain	Res	Type
7	B	330	C
7	B	347	G
7	B	352	C
7	B	354	G
7	B	367	U
7	B	369	G
7	B	372	C
7	B	376	G
7	B	392	C
7	B	393	A
7	B	397	A
7	B	404	G
7	B	406	G
7	B	412	A
7	B	413	G
7	B	414	A
7	B	421	U
7	B	422	C
7	B	423	G
7	B	424	G
7	B	429	U
7	B	435	A
7	B	446	G
7	B	451	A
7	B	453	G
7	B	457	G
7	B	467	U
7	B	468	A
7	B	469	C
7	B	479	U
7	B	484	G
7	B	486	U
7	B	500	G
7	B	511	C
7	B	518	C
7	B	519	C
7	B	521	G
7	B	547	A
7	B	559	A
7	B	572	A
7	B	573	A
7	B	575	G

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Mol	Chain	Res	Type
7	B	576	C
7	B	579	A
7	B	596	A
7	B	614	C
7	B	615	G
7	B	639	G
7	B	649	A
7	B	650	G
7	B	653	U
7	B	654	G
7	B	661	G
7	B	665	A
7	B	671	G
7	B	682	G
7	B	723	U
7	B	724	G
7	B	734	G
7	B	747	A
7	B	748	G
7	B	755	G
7	B	777	A
7	B	793	U
7	B	794	A
7	B	815	A
7	B	817	C
7	B	851	G
7	B	857	C
7	B	884	U
7	B	885	G
7	B	890	G
7	B	914	A
7	B	926	G
7	B	931	C
7	B	934	C
7	B	935	A
7	B	936	C
7	B	960	U
7	B	966	2MG
7	B	968	A
7	B	969	A
7	B	971	G
7	B	975	A

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Mol	Chain	Res	Type
7	B	976	G
7	B	977	A
7	B	978	A
7	B	984	C
7	B	992	U
7	B	993	G
7	B	994	A
7	B	996	A
7	B	1003	G
7	B	1004	A
7	B	1005	A
7	B	1008	U
7	B	1020	G
7	B	1023	U
7	B	1026	G
7	B	1027	C
7	B	1030	U
7	B	1031	C
7	B	1032	G
7	B	1033	G
7	B	1034	G
7	B	1036	A
7	B	1037	C
7	B	1039	G
7	B	1042	A
7	B	1044	A
7	B	1053	G
7	B	1060	U
7	B	1065	U
7	B	1070	U
7	B	1085	U
7	B	1094	G
7	B	1095	U
7	B	1101	A
7	B	1124	G
7	B	1125	U
7	B	1132	C
7	B	1135	U
7	B	1136	C
7	B	1137	C
7	B	1139	G
7	B	1159	U

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Mol	Chain	Res	Type
7	B	1169	A
7	B	1171	A
7	B	1174	G
7	B	1184	G
7	B	1187	G
7	B	1196	A
7	B	1197	A
7	B	1213	A
7	B	1214	C
7	B	1221	G
7	B	1225	A
7	B	1226	C
7	B	1227	A
7	B	1228	C
7	B	1238	A
7	B	1247	U
7	B	1248	A
7	B	1256	A
7	B	1257	A
7	B	1260	G
7	B	1274	A
7	B	1275	A
7	B	1280	A
7	B	1287	A
7	B	1300	G
7	B	1302	C
7	B	1312	G
7	B	1317	C
7	B	1319	A
7	B	1320	C
7	B	1338	G
7	B	1340	A
7	B	1346	A
7	B	1353	G
7	B	1363	A
7	B	1364	U
7	B	1370	G
7	B	1378	C
7	B	1379	G
7	B	1381	U
7	B	1419	G
7	B	1429	A

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Mol	Chain	Res	Type
7	B	1441	A
7	B	1450	U
7	B	1452	C
7	B	1453	G
7	B	1487	G
7	B	1497	G
7	B	1505	G
7	B	1506	U
7	B	1517	G
7	B	1529	G
7	B	1530	G
7	B	1534	A
29	X	14	A
29	X	17	C
29	X	18	G
29	X	19	G
29	X	21	A
29	X	22	G
29	X	42	C
29	X	43	C
29	X	46	G
29	X	47	U
29	X	48	C
29	X	51	U
29	X	60	U
29	X	62	C
29	X	64	A
29	X	65	G
29	X	75	C
29	X	76	A
31	Z	3	C
31	Z	4	C
31	Z	8	U
31	Z	9	A
31	Z	10	G
31	Z	11	C
31	Z	12	U
31	Z	13	C
31	Z	14	A
31	Z	15	G
31	Z	16	U
31	Z	17	G

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Mol	Chain	Res	Type
31	Z	18	G
31	Z	19	U
31	Z	20	U
31	Z	21	A
31	Z	26	A
31	Z	29	C
31	Z	30	G
31	Z	34	U
31	Z	37	A
31	Z	38	A
31	Z	39	U
31	Z	40	C
31	Z	43	U
31	Z	45	G
31	Z	47	U
31	Z	48	C
31	Z	49	G
31	Z	50	C
31	Z	52	G
31	Z	53	G
31	Z	58	A
31	Z	59	G
31	Z	60	U
31	Z	61	C
31	Z	65	C
31	Z	68	G
31	Z	69	G
31	Z	71	C
31	Z	76	A
32	a	10	A
32	a	34	U
32	a	42	A
32	a	45	G
32	a	71	A
32	a	74	A
32	a	75	G
32	a	84	A
32	a	101	A
32	a	102	U
32	a	110	G
32	a	118	A
32	a	119	A

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Mol	Chain	Res	Type
32	a	120	U
32	a	135	U
32	a	139	U
32	a	140	C
32	a	142	A
32	a	163	C
32	a	164	C
32	a	165	A
32	a	181	A
32	a	196	A
32	a	199	A
32	a	200	U
32	a	215	G
32	a	216	A
32	a	221	A
32	a	222	A
32	a	233	A
32	a	248	G
32	a	272	A
32	a	276	U
32	a	278	A
32	a	282	A
32	a	285	G
32	a	289	G
32	a	311	A
32	a	321	U
32	a	322	A
32	a	329	G
32	a	330	A
32	a	345	A
32	a	353	C
32	a	361	G
32	a	362	A
32	a	367	G
32	a	383	C
32	a	386	G
32	a	396	G
32	a	404	A
32	a	405	U
32	a	411	G
32	a	412	A
32	a	420	C

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Mol	Chain	Res	Type
32	a	425	G
32	a	451	U
32	a	481	G
32	a	489	G
32	a	490	C
32	a	491	G
32	a	505	A
32	a	508	A
32	a	509	C
32	a	530	G
32	a	531	C
32	a	532	A
32	a	533	G
32	a	545	U
32	a	546	U
32	a	547	A
32	a	549	G
32	a	563	A
32	a	573	U
32	a	575	A
32	a	586	A
32	a	603	A
32	a	614	A
32	a	615	U
32	a	618	G
32	a	627	A
32	a	637	A
32	a	645	C
32	a	647	G
32	a	653	U
32	a	654	A
32	a	655	A
32	a	659	G
32	a	668	A
32	a	685	A
32	a	686	U
32	a	717	C
32	a	724	U
32	a	730	A
32	a	738	G
32	a	747	5MU
32	a	764	A

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Mol	Chain	Res	Type
32	a	765	C
32	a	775	G
32	a	776	G
32	a	777	G
32	a	782	A
32	a	784	G
32	a	785	G
32	a	792	A
32	a	805	G
32	a	812	C
32	a	827	U
32	a	828	U
32	a	845	A
32	a	846	U
32	a	858	G
32	a	859	G
32	a	869	G
32	a	879	G
32	a	881	G
32	a	883	G
32	a	888	C
32	a	890	C
32	a	891	G
32	a	893	C
32	a	895	U
32	a	896	A
32	a	897	C
32	a	907	G
32	a	910	A
32	a	914	G
32	a	915	C
32	a	931	U
32	a	934	U
32	a	946	C
32	a	961	C
32	a	962	G
32	a	974	G
32	a	983	A
32	a	984	A
32	a	985	C
32	a	996	A
32	a	1005	C

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Mol	Chain	Res	Type
32	a	1012	U
32	a	1013	C
32	a	1022	G
32	a	1026	G
32	a	1033	U
32	a	1040	A
32	a	1046	A
32	a	1047	G
32	a	1108	U
32	a	1109	C
32	a	1111	A
32	a	1112	G
32	a	1116	G
32	a	1119	U
32	a	1128	G
32	a	1129	A
32	a	1132	U
32	a	1133	A
32	a	1135	C
32	a	1142	A
32	a	1171	G
32	a	1179	G
32	a	1187	G
32	a	1205	A
32	a	1250	G
32	a	1253	A
32	a	1256	G
32	a	1271	G
32	a	1272	A
32	a	1286	A
32	a	1287	A
32	a	1300	G
32	a	1301	A
32	a	1320	C
32	a	1321	A
32	a	1329	U
32	a	1352	U
32	a	1365	A
32	a	1379	U
32	a	1383	A
32	a	1416	G
32	a	1428	C

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Mol	Chain	Res	Type
32	a	1434	A
32	a	1452	G
32	a	1453	A
32	a	1482	G
32	a	1490	A
32	a	1491	G
32	a	1493	C
32	a	1504	A
32	a	1508	A
32	a	1510	G
32	a	1515	A
32	a	1529	G
32	a	1531	C
32	a	1534	U
32	a	1535	A
32	a	1536	C
32	a	1537	G
32	a	1538	G
32	a	1542	U
32	a	1569	A
32	a	1578	U
32	a	1583	A
32	a	1584	U
32	a	1585	C
32	a	1593	A
32	a	1608	A
32	a	1609	A
32	a	1622	G
32	a	1647	U
32	a	1648	U
32	a	1649	G
32	a	1674	G
32	a	1715	G
32	a	1729	U
32	a	1730	C
32	a	1731	G
32	a	1732	C
32	a	1733	G
32	a	1738	G
32	a	1739	A
32	a	1750	G
32	a	1764	C

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Mol	Chain	Res	Type
32	a	1773	A
32	a	1800	C
32	a	1801	A
32	a	1807	G
32	a	1808	A
32	a	1816	C
32	a	1829	A
32	a	1841	U
32	a	1847	A
32	a	1848	A
32	a	1858	A
32	a	1862	G
32	a	1866	A
32	a	1870	C
32	a	1871	A
32	a	1872	A
32	a	1873	G
32	a	1905	C
32	a	1906	G
32	a	1907	G
32	a	1913	A
32	a	1929	G
32	a	1930	G
32	a	1937	A
32	a	1938	A
32	a	1955	U
32	a	1965	C
32	a	1967	C
32	a	1970	A
32	a	1971	U
32	a	1972	G
32	a	1987	A
32	a	1991	U
32	a	1993	U
32	a	2023	C
32	a	2030	A
32	a	2031	A
32	a	2033	A
32	a	2043	C
32	a	2055	C
32	a	2056	G
32	a	2060	A

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Mol	Chain	Res	Type
32	a	2061	G
32	a	2069	G7M
32	a	2077	A
32	a	2093	G
32	a	2192	U
32	a	2198	A
32	a	2203	U
32	a	2204	G
32	a	2211	A
32	a	2223	G
32	a	2225	A
32	a	2238	G
32	a	2268	A
32	a	2282	G
32	a	2283	C
32	a	2287	A
32	a	2305	U
32	a	2308	G
32	a	2312	U
32	a	2322	A
32	a	2325	G
32	a	2333	A
32	a	2335	A
32	a	2347	C
32	a	2350	C
32	a	2361	G
32	a	2372	U
32	a	2383	G
32	a	2385	C
32	a	2396	G
32	a	2402	U
32	a	2403	C
32	a	2406	A
32	a	2425	A
32	a	2429	G
32	a	2430	A
32	a	2435	A
32	a	2441	U
32	a	2447	G
32	a	2448	A
32	a	2474	U
32	a	2476	A

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Mol	Chain	Res	Type
32	a	2480	C
32	a	2502	G
32	a	2505	G
32	a	2506	U
32	a	2518	A
32	a	2529	G
32	a	2535	G
32	a	2547	A
32	a	2554	U
32	a	2566	A
32	a	2567	G
32	a	2573	C
32	a	2574	G
32	a	2602	A
32	a	2603	G
32	a	2613	U
32	a	2629	U
32	a	2630	G
32	a	2663	G
32	a	2671	G
32	a	2682	A
32	a	2689	U
32	a	2690	U
32	a	2714	G
32	a	2726	A
32	a	2744	G
32	a	2748	A
32	a	2757	A
32	a	2758	A
32	a	2765	A
32	a	2778	A
32	a	2798	U
32	a	2800	A
32	a	2820	A
32	a	2821	A
32	a	2880	C
32	a	2884	U
32	a	2885	G
32	a	2891	U
32	a	2899	A
32	a	2901	C
33	b	9	G

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Mol	Chain	Res	Type
33	b	17	C
33	b	25	U
33	b	34	A
33	b	42	C
33	b	45	A
33	b	56	G
33	b	89	U
33	b	90	C
33	b	99	A
33	b	105	G
33	b	109	A
33	b	119	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	B	7	A
7	B	65	A
7	B	70	U
7	B	83	C
7	B	119	A
7	B	214	C
7	B	251	G
7	B	266	G
7	B	329	A
7	B	468	A
7	B	559	A
7	B	575	G
7	B	653	U
7	B	793	U
7	B	884	U
7	B	992	U
7	B	993	G
7	B	1026	G
7	B	1035	A
7	B	1129	C
7	B	1136	C
7	B	1225	A
7	B	1319	A
7	B	1445	U
29	X	16	U
29	X	18	G

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Mol	Chain	Res	Type
29	X	60	U
29	X	74	C
31	Z	9	A
31	Z	20	U
31	Z	39	U

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

32 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	$\# Z > 2$
32	PSU	a	2605	32	18,21,22	1.70	1 (5%)	22,30,33	0.78	1 (4%)
32	5MU	a	747	32	19,22,23	0.31	0	28,32,35	0.46	0
32	1MG	a	745	32	22,26,27	0.51	0	33,39,42	0.53	0
32	PSU	a	955	32	18,21,22	0.93	1 (5%)	22,30,33	0.83	1 (4%)
32	OMG	a	2251	32,60,29	23,26,27	0.30	0	33,38,41	0.41	0
32	PSU	a	2457	32	18,21,22	1.11	1 (5%)	22,30,33	0.64	0
32	PSU	a	1911	32	18,21,22	0.92	1 (5%)	22,30,33	0.67	0
32	5MU	a	1939	32	19,22,23	0.33	0	28,32,35	0.50	0
32	OMC	a	2498	32,60	19,22,23	0.29	0	26,31,34	0.56	0
7	5MC	B	967	7	18,22,23	0.29	0	26,32,35	0.56	0
32	2MA	a	2503	32,60	22,25,26	0.79	1 (4%)	33,37,40	1.10	3 (9%)
7	4OC	B	1402	7	20,23,24	0.45	0	26,32,35	0.58	0
32	PSU	a	2604	32	18,21,22	1.01	1 (5%)	22,30,33	0.96	1 (4%)
7	2MG	B	1516	7	23,26,27	0.41	0	32,38,41	0.51	0
35	MEQ	d	150	35	8,9,10	0.47	0	5,10,12	0.72	0
32	PSU	a	1917	32	18,21,22	0.88	1 (5%)	22,30,33	0.65	0
7	5MC	B	1407	7	18,22,23	0.31	0	26,32,35	0.70	0
32	PSU	a	746	32,60	18,21,22	0.88	1 (5%)	22,30,33	0.79	0
7	2MG	B	966	7	23,26,27	0.38	0	32,38,41	0.41	0
7	UR3	B	1498	7	19,22,23	0.33	0	26,32,35	0.62	0
32	2MG	a	2445	32	23,26,27	0.49	0	32,38,41	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PSU	a	2504	32	18,21,22	0.95	1 (5%)	22,30,33	0.65	0
32	5MC	a	1962	32	18,22,23	0.37	0	26,32,35	0.52	0
7	2MG	B	1207	7	23,26,27	0.36	0	32,38,41	0.48	0
7	PSU	B	516	7	18,21,22	0.95	1 (5%)	22,30,33	0.63	0
32	6MZ	a	1618	32	22,25,26	2.93	1 (4%)	30,36,39	1.45	1 (3%)
32	OMU	a	2552	32	19,22,23	0.24	0	26,31,34	0.57	0
32	2MG	a	1835	32	23,26,27	0.81	1 (4%)	32,38,41	0.53	0
32	PSU	a	2580	32,60	18,21,22	1.07	1 (5%)	22,30,33	0.82	1 (4%)
32	H2U	a	2449	32	18,21,22	0.55	0	21,30,33	0.86	1 (4%)
7	G7M	B	527	7	23,26,27	0.74	1 (4%)	35,39,42	0.63	1 (2%)
32	G7M	a	2069	32	23,26,27	1.14	1 (4%)	35,39,42	0.69	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
32	PSU	a	2605	32	-	0/7/25/26	0/2/2/2
32	5MU	a	747	32	-	2/7/25/26	0/2/2/2
32	1MG	a	745	32	-	0/7/25/26	0/3/3/3
32	PSU	a	955	32	-	0/7/25/26	0/2/2/2
32	OMG	a	2251	32,60,29	-	1/9/27/28	0/3/3/3
32	PSU	a	2457	32	-	0/7/25/26	0/2/2/2
32	PSU	a	1911	32	-	0/7/25/26	0/2/2/2
32	5MU	a	1939	32	-	0/7/25/26	0/2/2/2
32	OMC	a	2498	32,60	-	0/9/27/28	0/2/2/2
7	5MC	B	967	7	-	0/7/25/26	0/2/2/2
32	2MA	a	2503	32,60	-	3/7/25/26	0/3/3/3
7	4OC	B	1402	7	-	1/9/29/30	0/2/2/2
32	PSU	a	2604	32	-	0/7/25/26	0/2/2/2
7	2MG	B	1516	7	-	0/9/27/28	0/3/3/3
35	MEQ	d	150	35	-	2/8/9/11	-
32	PSU	a	1917	32	-	0/7/25/26	0/2/2/2
7	5MC	B	1407	7	-	0/7/25/26	0/2/2/2
32	PSU	a	746	32,60	-	2/7/25/26	0/2/2/2
7	2MG	B	966	7	-	2/9/27/28	0/3/3/3
7	UR3	B	1498	7	-	0/7/25/26	0/2/2/2
32	2MG	a	2445	32	-	0/9/27/28	0/3/3/3
32	PSU	a	2504	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	a	1962	32	-	2/7/25/26	0/2/2/2
7	2MG	B	1207	7	-	2/9/27/28	0/3/3/3
7	PSU	B	516	7	-	0/7/25/26	0/2/2/2
32	6MZ	a	1618	32	-	0/9/27/28	0/3/3/3
32	OMU	a	2552	32	-	0/9/27/28	0/2/2/2
32	2MG	a	1835	32	-	0/9/27/28	0/3/3/3
32	PSU	a	2580	32,60	-	0/7/25/26	0/2/2/2
32	H2U	a	2449	32	-	0/7/38/39	0/2/2/2
7	G7M	B	527	7	-	0/7/25/26	0/3/3/3
32	G7M	a	2069	32	-	2/7/25/26	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	1618	6MZ	C9-N6	13.52	1.68	1.45
32	a	2605	PSU	C6-C5	6.57	1.43	1.35
32	a	2457	PSU	C6-C5	4.30	1.40	1.35
32	a	2580	PSU	C6-C5	4.13	1.40	1.35
32	a	2069	G7M	C8-N7	4.01	1.40	1.33
7	B	516	PSU	C6-C5	3.66	1.39	1.35
32	a	1911	PSU	C6-C5	3.55	1.39	1.35
32	a	2504	PSU	C6-C5	3.53	1.39	1.35
32	a	1835	2MG	CM2-N2	3.45	1.51	1.45
32	a	955	PSU	C6-C5	3.42	1.39	1.35
32	a	1917	PSU	C6-C5	3.38	1.39	1.35
32	a	2604	PSU	C6-C5	3.38	1.39	1.35
32	a	746	PSU	C6-C5	3.29	1.39	1.35
7	B	527	G7M	C8-N7	2.55	1.37	1.33
32	a	2503	2MA	C6-N6	-2.40	1.28	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1618	6MZ	C9-N6-C6	-7.05	116.80	122.87
32	a	2503	2MA	C5-C4-N3	-2.89	123.94	127.19
32	a	2449	H2U	C4-N3-C2	-2.62	123.62	125.79
32	a	2580	PSU	C3'-C2'-C1'	2.53	104.59	101.64
32	a	2503	2MA	C2-N1-C6	2.50	121.97	118.08
32	a	2604	PSU	C2'-C3'-C4'	-2.44	97.90	102.64
32	a	2605	PSU	C2'-C3'-C4'	-2.38	98.02	102.64
32	a	2503	2MA	N3-C2-N1	-2.10	121.86	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	955	PSU	C5-C6-N1	-2.05	119.03	122.11
7	B	527	G7M	N9-C8-N7	-2.04	107.16	112.21

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	966	2MG	O4'-C4'-C5'-O5'
7	B	966	2MG	C3'-C4'-C5'-O5'
7	B	1207	2MG	N1-C2-N2-CM2
7	B	1207	2MG	N3-C2-N2-CM2
32	a	746	PSU	C2'-C1'-C5-C4
32	a	2251	OMG	C1'-C2'-O2'-CM2
35	d	150	MEQ	NE2-CD-CG-CB
35	d	150	MEQ	OE1-CD-CG-CB
32	a	747	5MU	C3'-C4'-C5'-O5'
32	a	747	5MU	O4'-C4'-C5'-O5'
32	a	2069	G7M	C4'-C5'-O5'-P
32	a	1962	5MC	O4'-C1'-N1-C6
32	a	1962	5MC	C2'-C1'-N1-C6
32	a	2503	2MA	O4'-C1'-N9-C8
7	B	1402	4OC	O4'-C4'-C5'-O5'
32	a	746	PSU	O4'-C1'-C5-C6
32	a	2503	2MA	O4'-C4'-C5'-O5'
32	a	2069	G7M	O4'-C4'-C5'-O5'
32	a	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	a	2251	OMG	1	0
32	a	1939	5MU	1	0
7	B	1402	4OC	1	0
32	a	2604	PSU	1	0
7	B	1516	2MG	1	0
35	d	150	MEQ	1	0
32	a	1618	6MZ	3	0
7	B	527	G7M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 309 ligands modelled in this entry, 307 are monoatomic - leaving 2 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	$\# Z > 2$
61	SPM	a	6209	-	13,13,13	0.21	0	12,12,12	0.20	0
59	A2G	A	101	6	14,14,15	0.48	0	17,19,21	0.95	1 (5%)

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
61	SPM	a	6209	-	-	5/11/11/11	-
59	A2G	A	101	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	A	101	A2G	O5-C1-C2	-3.34	106.01	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	a	6209	SPM	C2-C3-C4-N5
61	a	6209	SPM	N5-C6-C7-C8
61	a	6209	SPM	C11-C12-C13-N14

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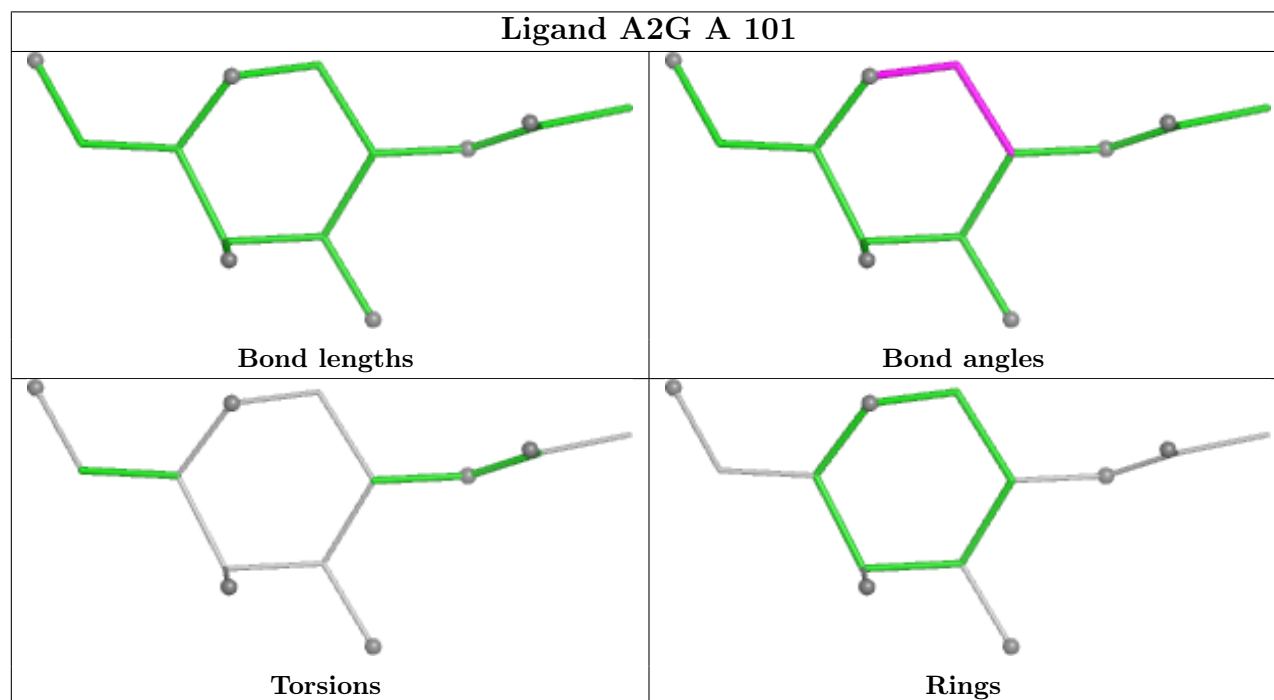
Mol	Chain	Res	Type	Atoms
61	a	6209	SPM	N1-C2-C3-C4
61	a	6209	SPM	N10-C11-C12-C13

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	a	6209	SPM	2	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

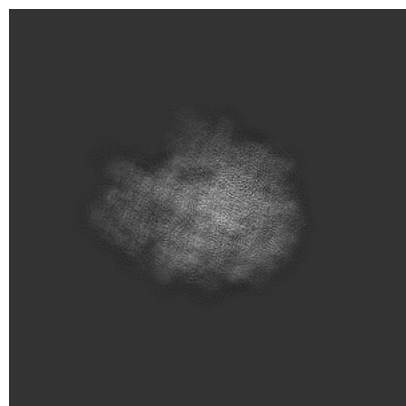
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15488. These allow visual inspection of the internal detail of the map and identification of artifacts.

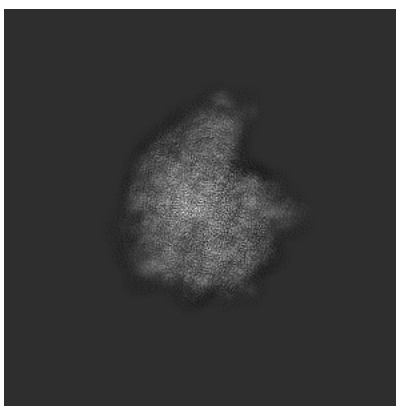
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

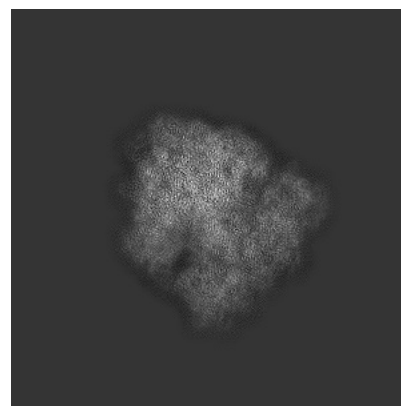
6.1.1 Primary map



X

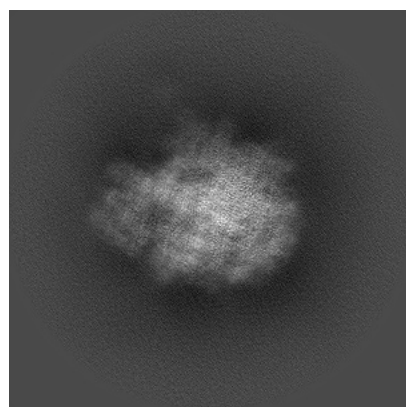


Y

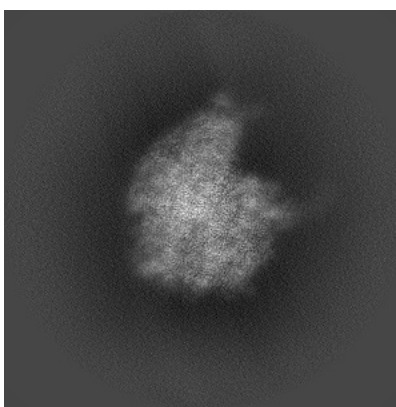


Z

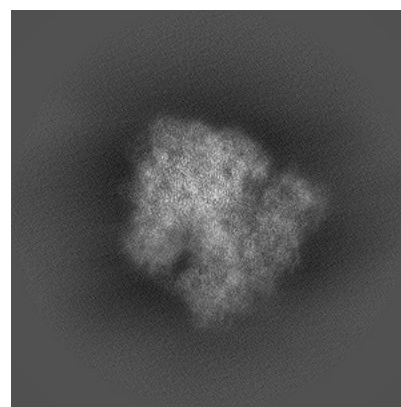
6.1.2 Raw map



X



Y

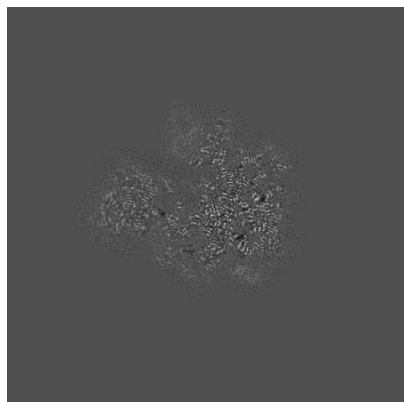


Z

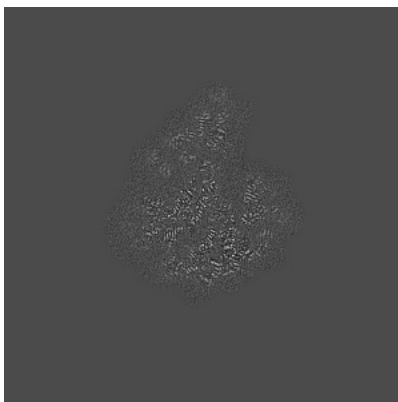
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

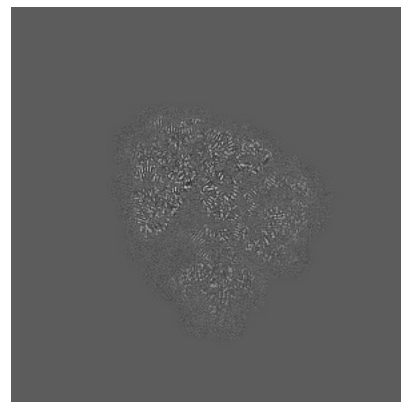
6.2.1 Primary map



X Index: 300

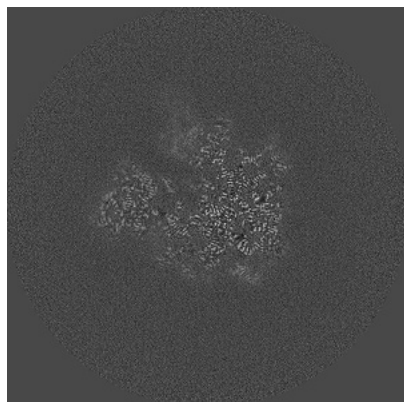


Y Index: 300

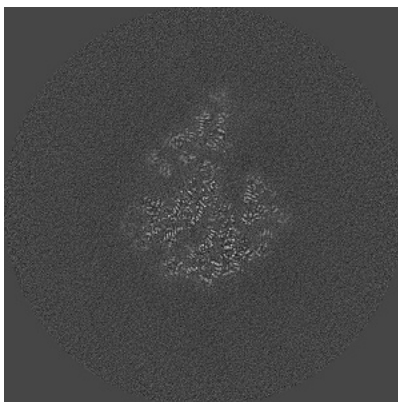


Z Index: 300

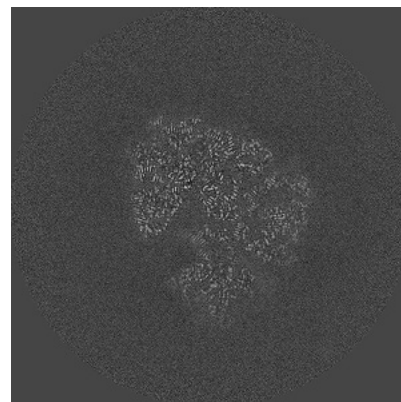
6.2.2 Raw map



X Index: 300



Y Index: 300

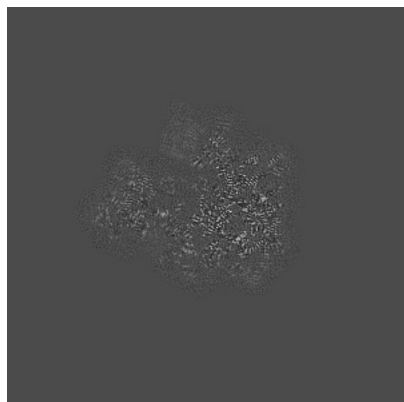


Z Index: 300

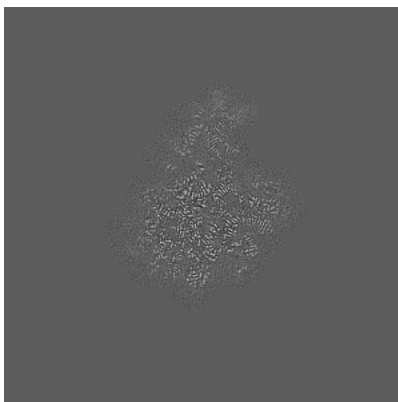
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

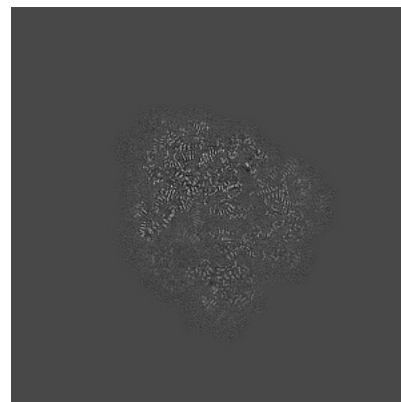
6.3.1 Primary map



X Index: 302

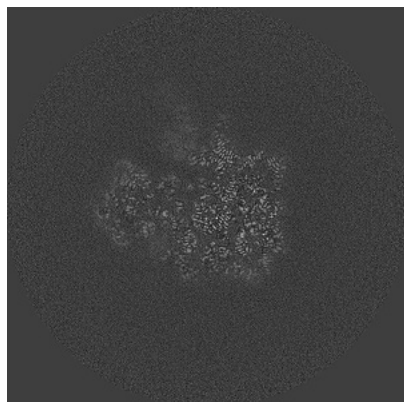


Y Index: 313

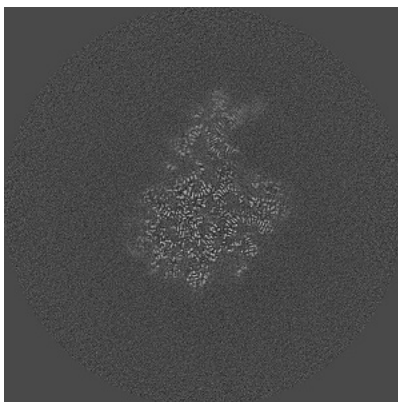


Z Index: 310

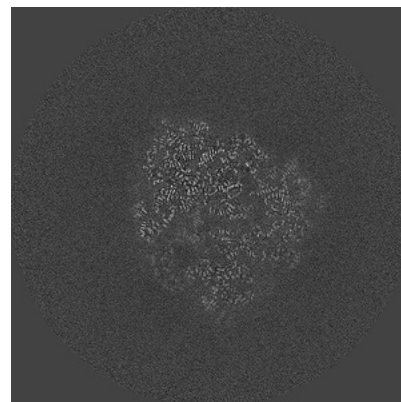
6.3.2 Raw map



X Index: 307



Y Index: 313

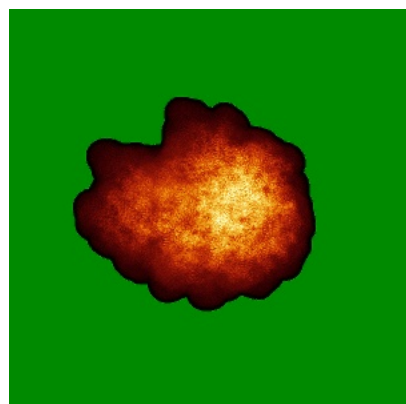


Z Index: 310

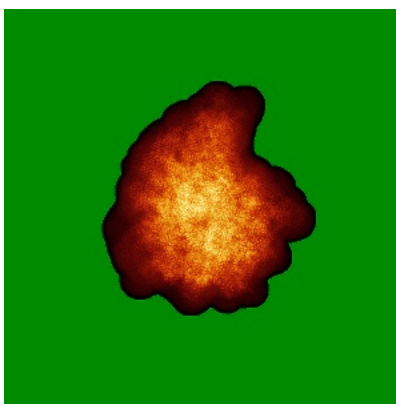
The images above show the largest variance slices of the map in three orthogonal directions.

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

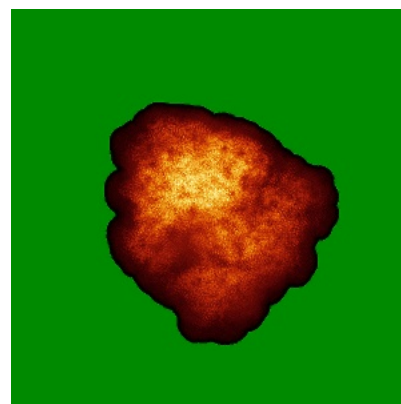
6.4.1 Primary map



X

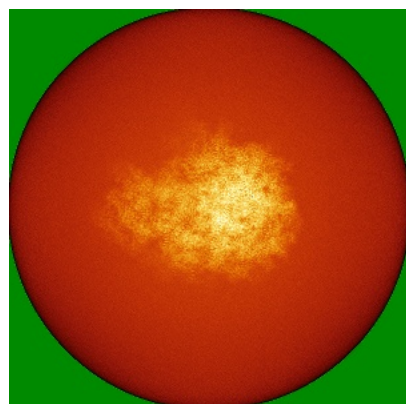


Y

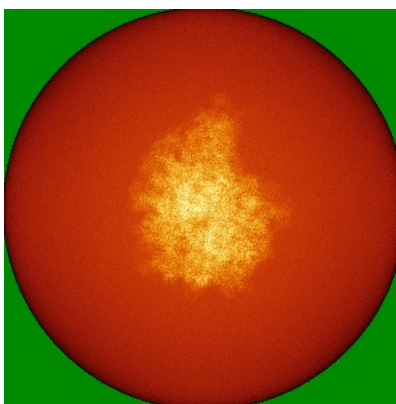


Z

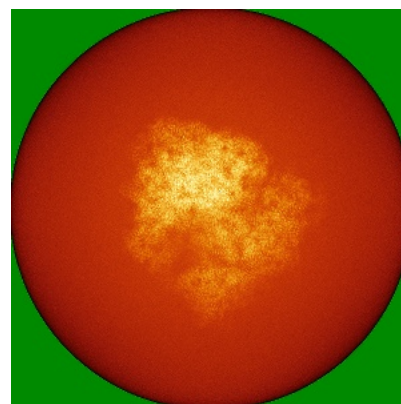
6.4.2 Raw map



X



Y

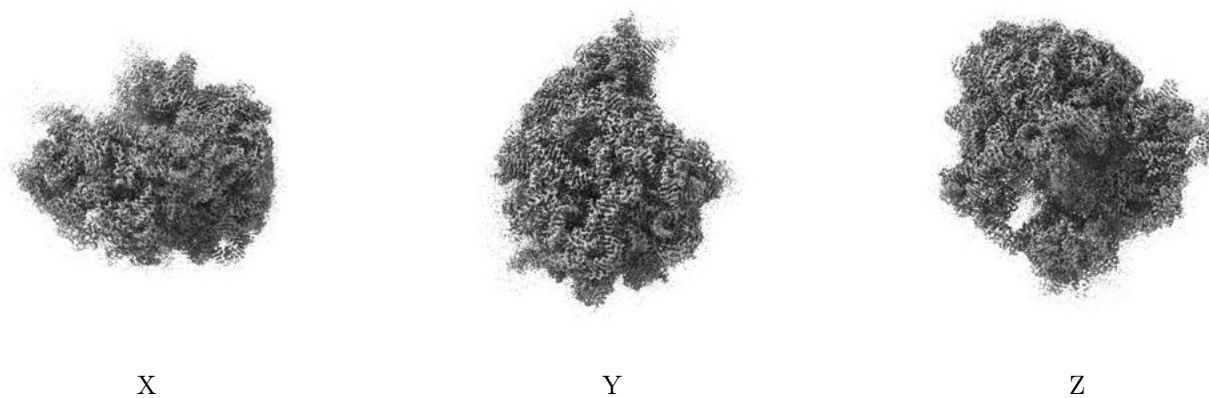


Z

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.

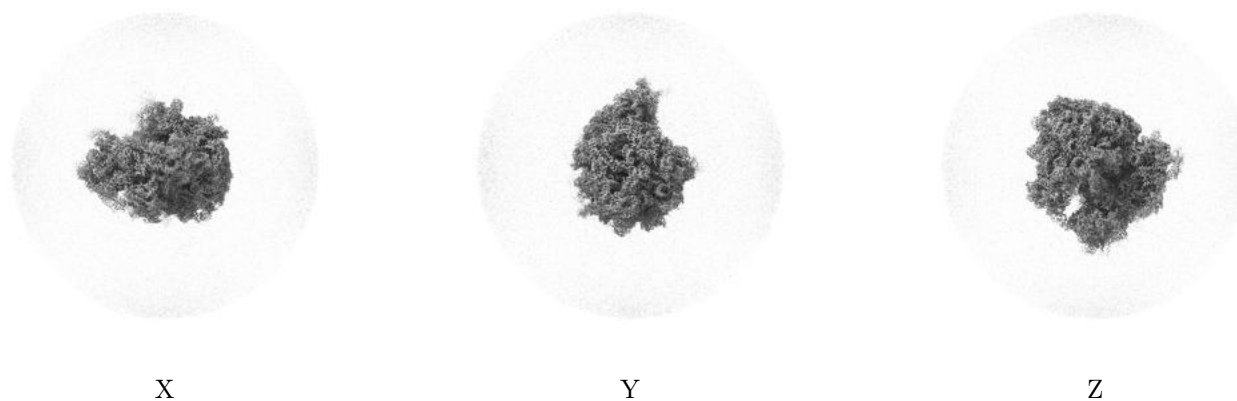
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



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

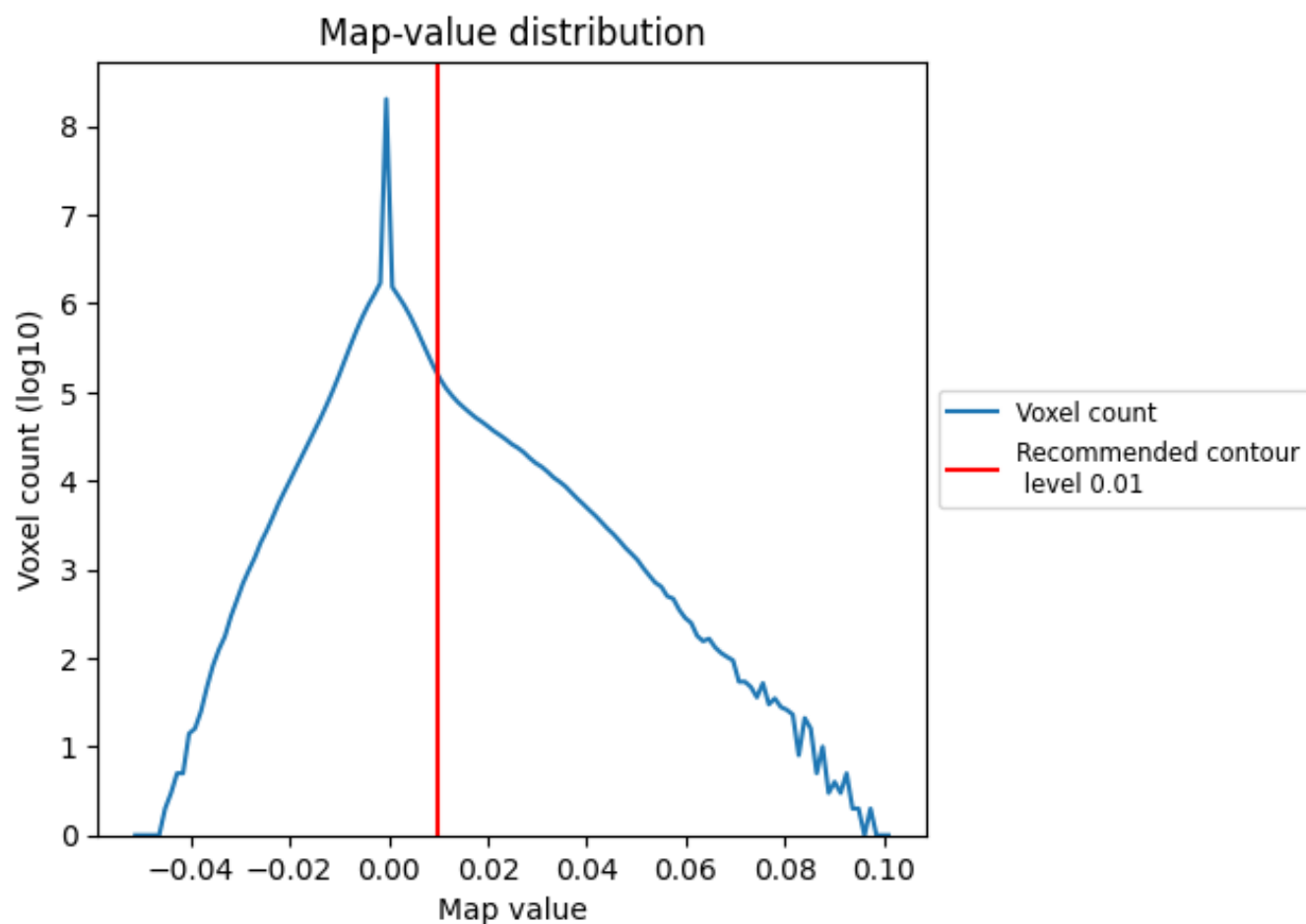
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

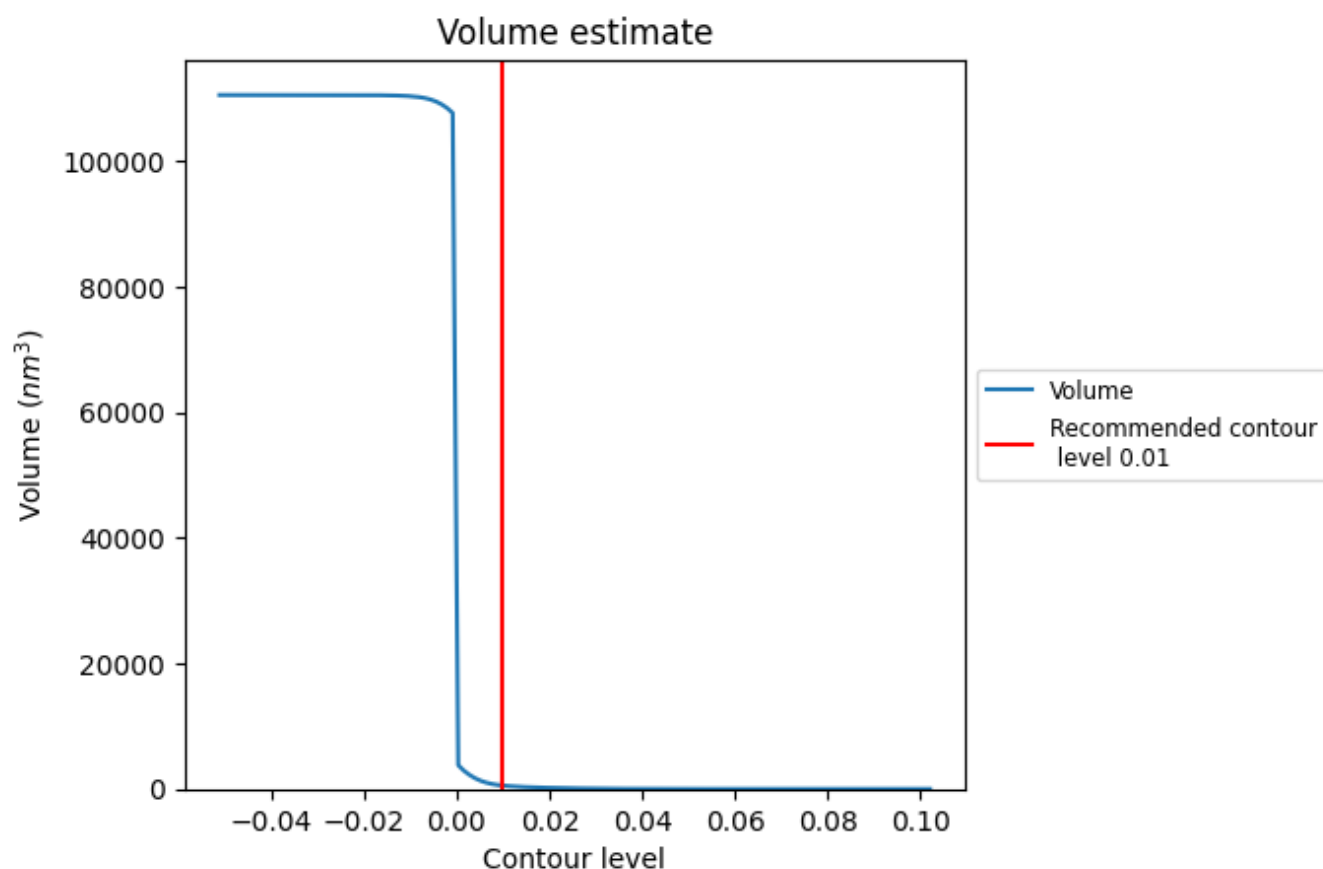
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

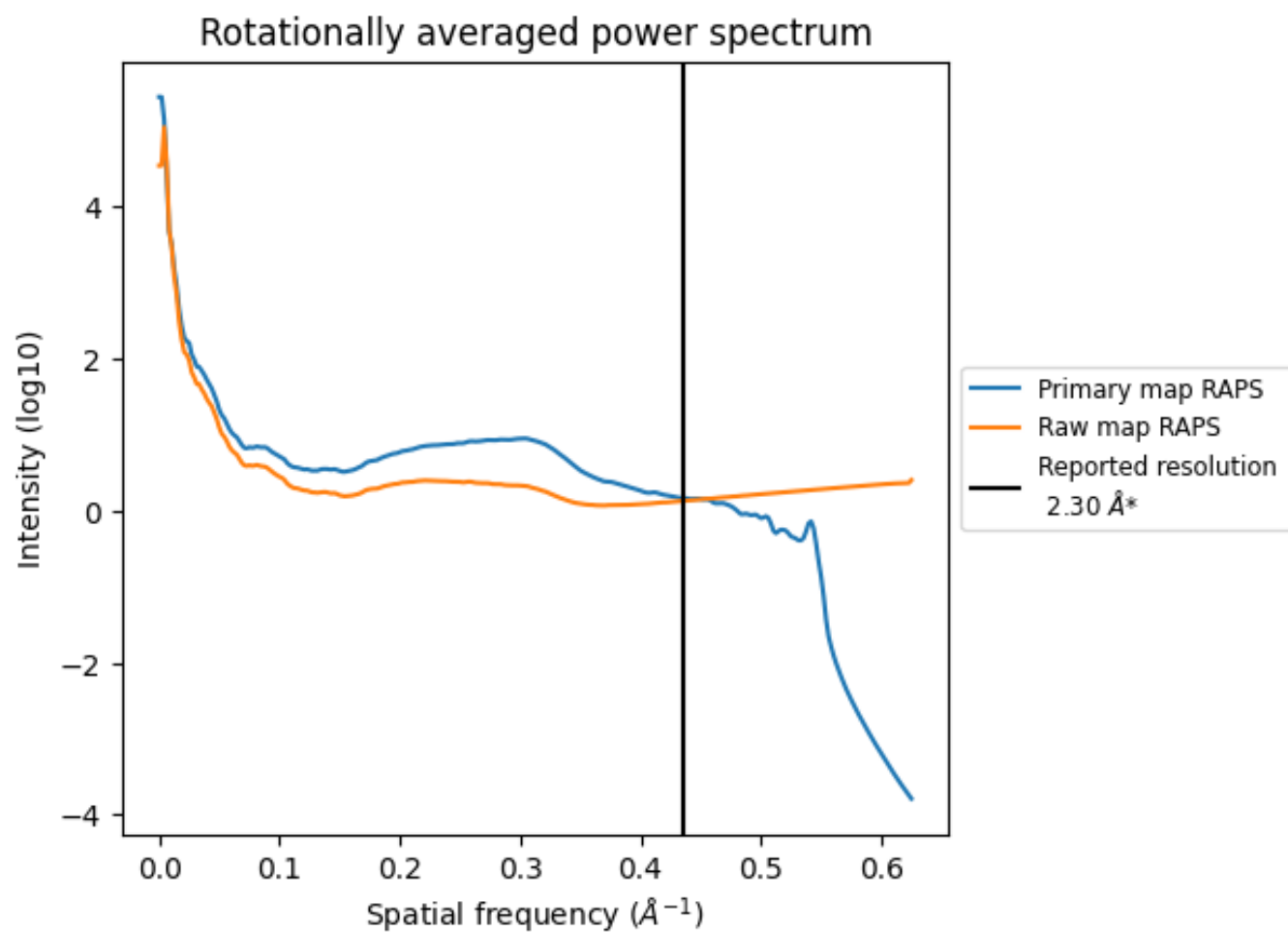
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 537 nm^3 ; this corresponds to an approximate mass of 485 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 ⓘ

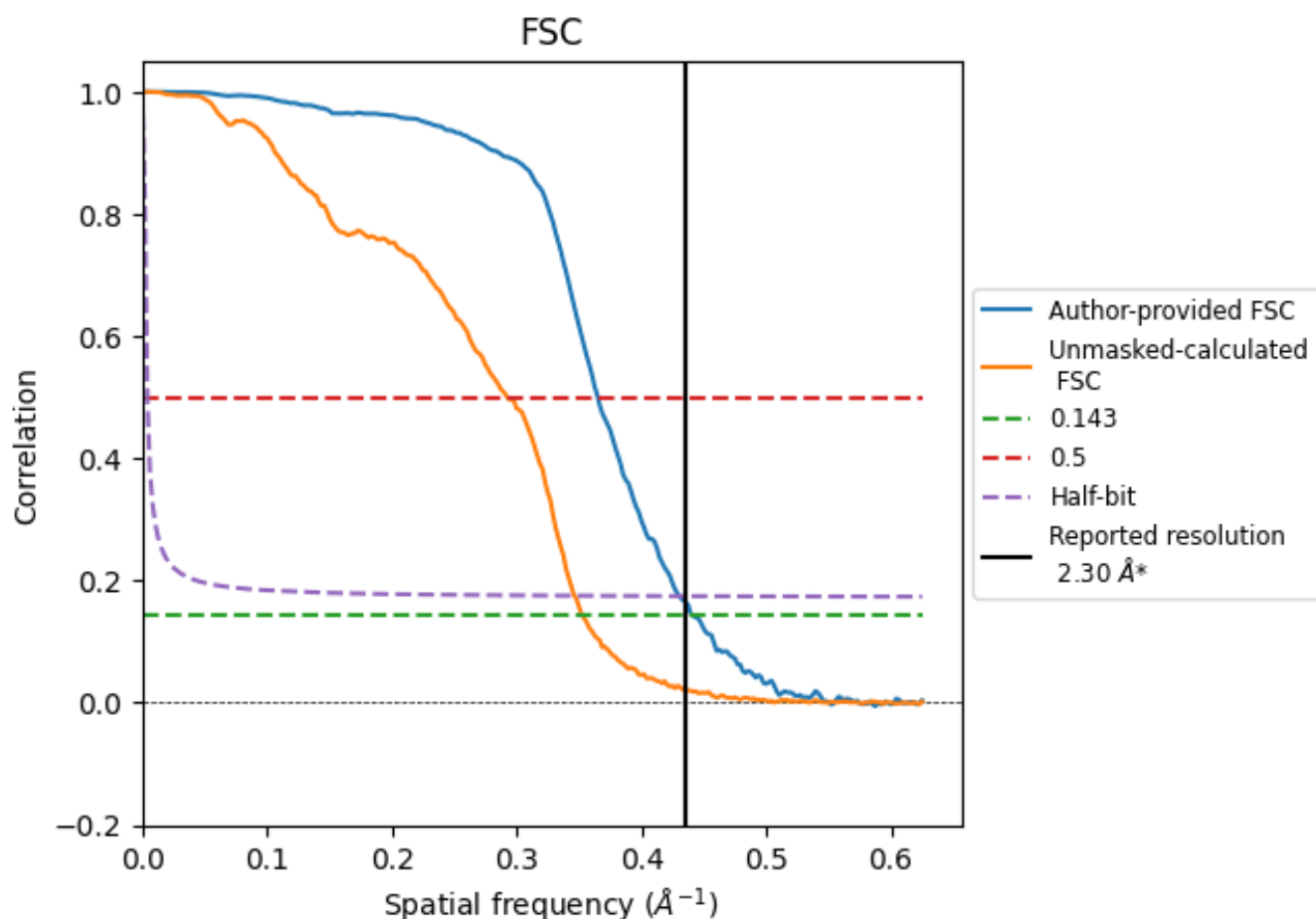


*Reported resolution corresponds to spatial frequency of $0.435 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.435 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

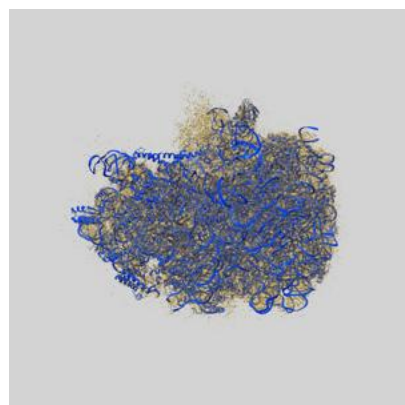
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.27	2.74	2.32
Unmasked-calculated*	2.84	3.42	2.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.84 differs from the reported value 2.3 by more than 10 %

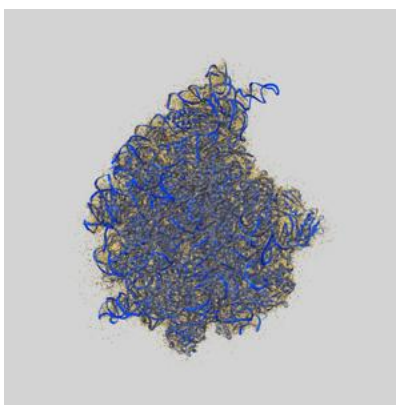
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15488 and PDB model 8AKN. Per-residue inclusion information can be found in section [3](#) on page [18](#).

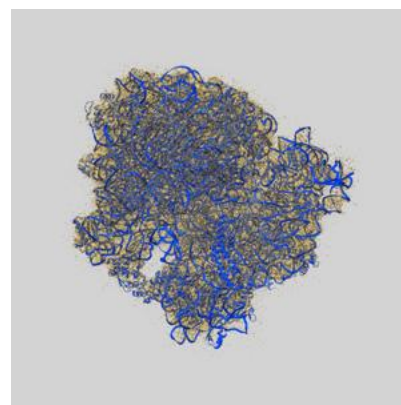
9.1 Map-model overlay [i](#)



X



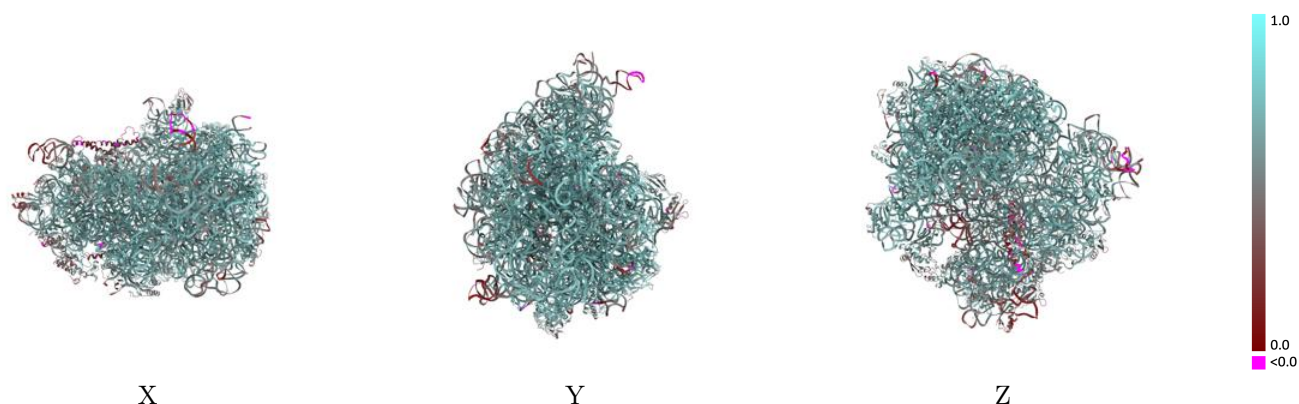
Y



Z

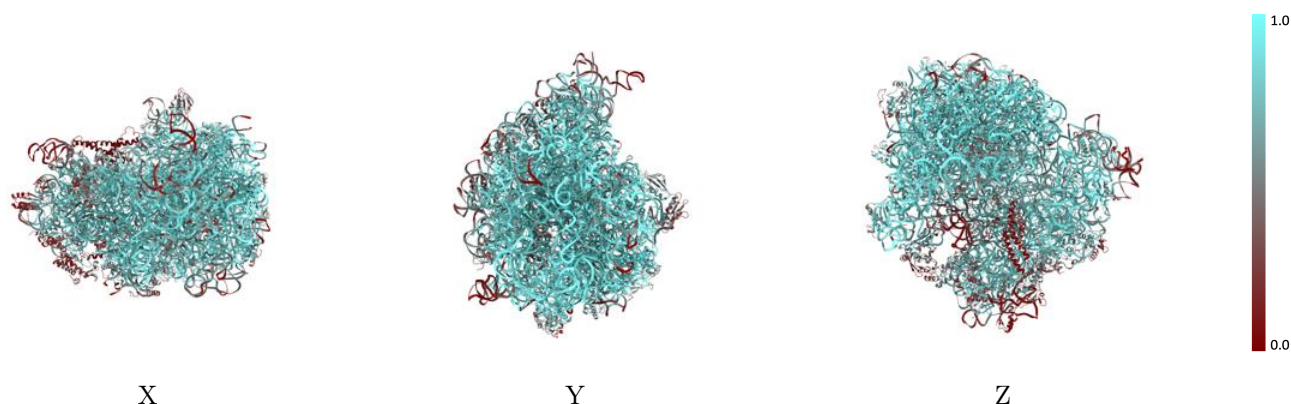
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



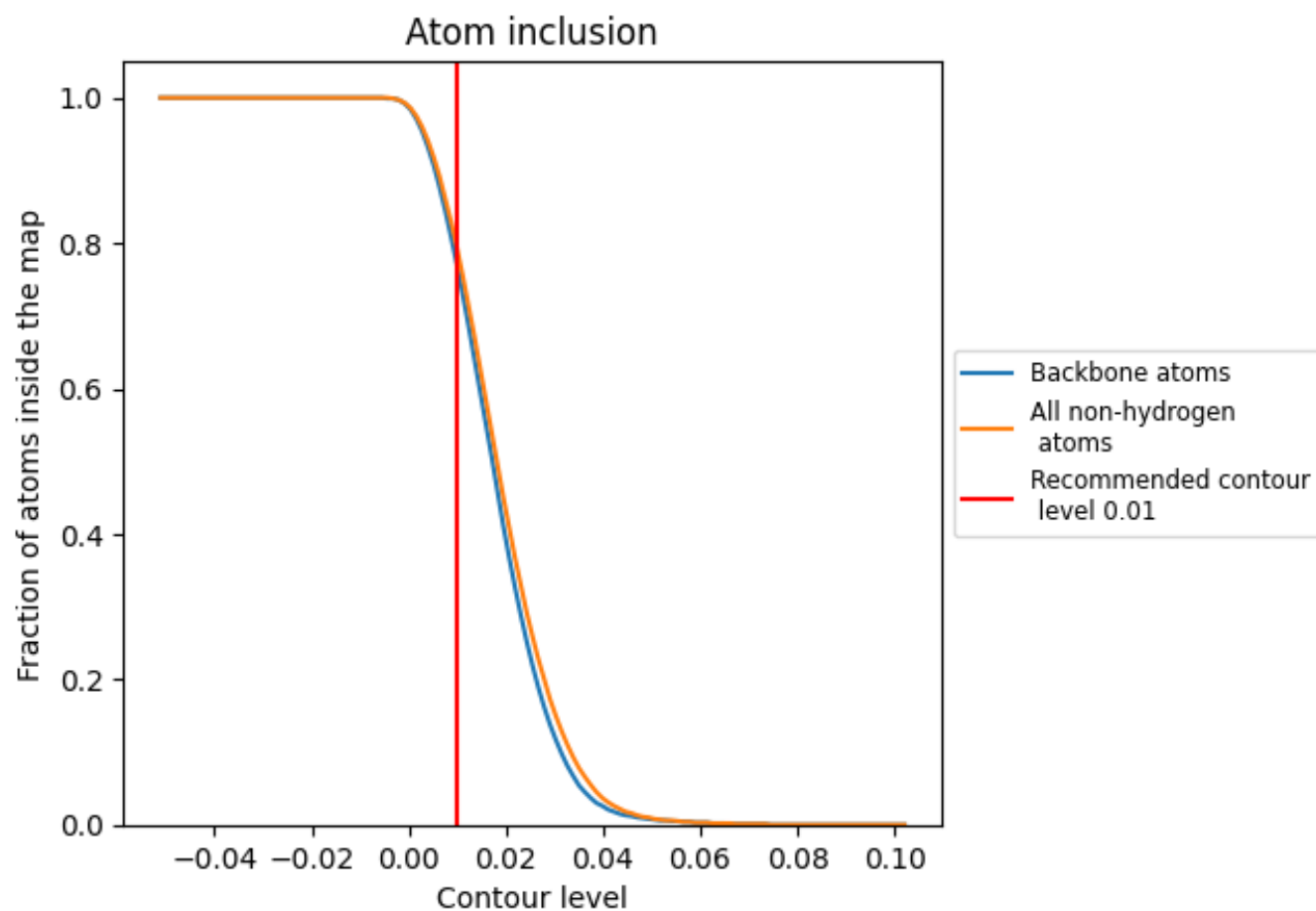
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7910	 0.6470
0	 0.7630	 0.6540
1	 0.9490	 0.7390
2	 0.9470	 0.7420
3	 0.8670	 0.7010
4	 0.2310	 0.4510
A	 0.9500	 0.7340
B	 0.8180	 0.6510
C	 0.3290	 0.4750
D	 0.6070	 0.5820
E	 0.5400	 0.5630
F	 0.7600	 0.6530
G	 0.4350	 0.5230
H	 0.4510	 0.5100
I	 0.7590	 0.6550
J	 0.5910	 0.5900
K	 0.4680	 0.4980
L	 0.6510	 0.6080
M	 0.7880	 0.6640
N	 0.5230	 0.5630
O	 0.6470	 0.6090
P	 0.6930	 0.6200
Q	 0.7260	 0.6270
R	 0.5840	 0.5720
S	 0.6440	 0.5910
T	 0.4970	 0.5490
U	 0.6990	 0.6170
V	 0.3920	 0.4400
W	 0.4800	 0.4850
X	 0.5660	 0.5470
Y	 0.8670	 0.6710
Z	 0.0880	 0.2320
a	 0.8890	 0.6860
b	 0.8310	 0.6460
c	 0.9110	 0.7240



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Chain	Atom inclusion	Q-score
d	 0.8800	 0.7150
e	 0.7260	 0.6450
f	 0.4920	 0.5430
g	 0.4730	 0.5120
h	 0.4630	 0.5130
i	 0.8860	 0.7080
j	 0.8420	 0.6970
k	 0.8230	 0.6830
l	 0.8700	 0.7070
m	 0.9460	 0.7370
n	 0.7510	 0.6390
o	 0.8480	 0.6920
p	 0.9220	 0.7330
q	 0.7540	 0.6560
r	 0.8610	 0.6930
s	 0.7150	 0.6120
t	 0.6170	 0.5630
u	 0.7100	 0.6280
v	 0.8790	 0.7020
w	 0.8270	 0.6690
x	 0.5870	 0.5660
y	 0.8440	 0.6750
z	 0.8140	 0.6810