



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 02:11 AM UTC

PDB ID : 7NHK / pdb_00007nhk
EMDB ID : EMD-12331
Title : LsaA, an antibiotic resistance ABCF, in complex with 70S ribosome from *Enterococcus faecalis*
Authors : Crowe-McAuliffe, C.; Kasari, M.; Hauryliuk, V.H.; Wilson, D.N.
Deposited on : 2021-02-10
Resolution : 2.90 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:

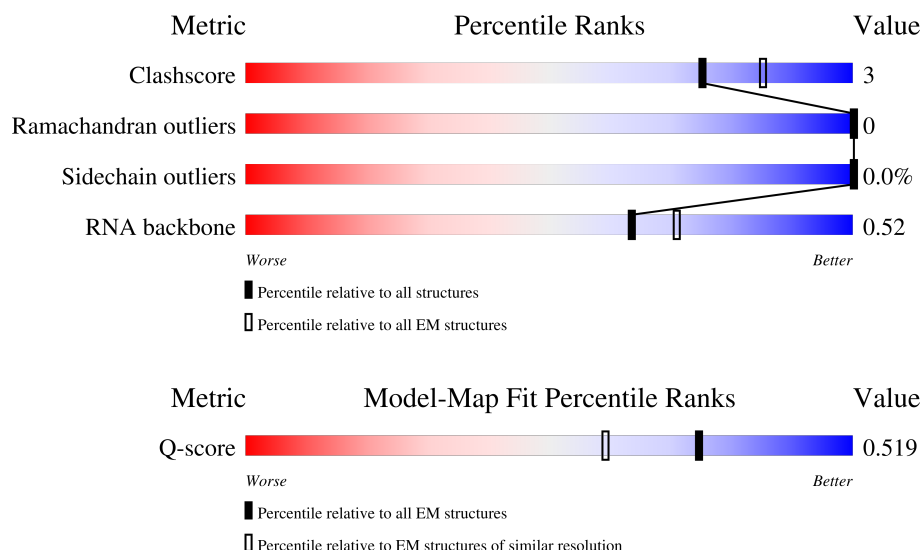
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.90 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.



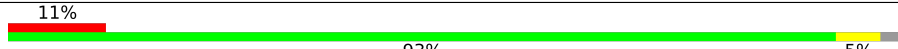
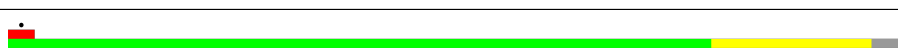
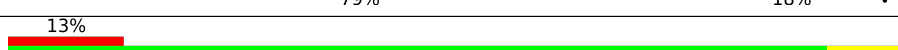
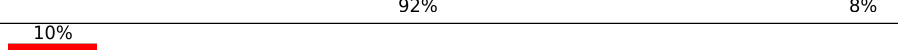
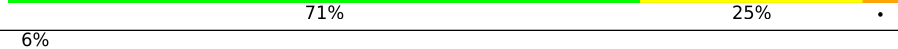
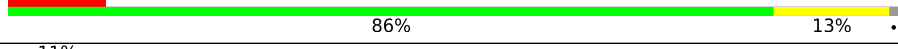
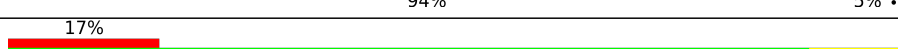
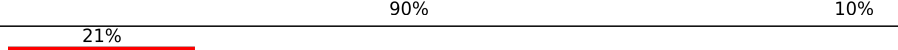
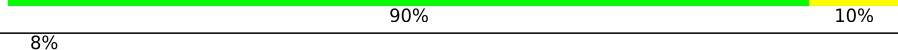
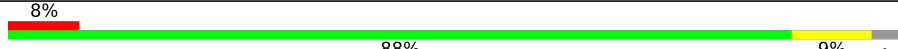
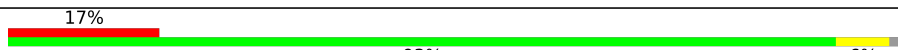
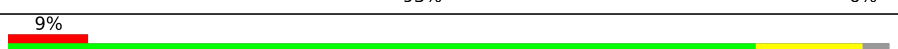
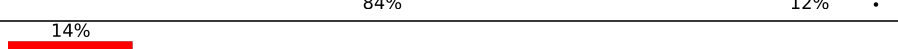
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	541	32% 84% 8% 9%
2	1	62	31% 79% 16% 5%
3	2	59	15% 85% 12% .

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Mol	Chain	Length	Quality of chain
4	4	59	
5	5	49	
6	6	44	
7	7	66	
8	8	38	
9	A	2912	
10	B	116	
11	G	276	
12	H	209	
13	I	207	
14	J	179	
15	K	178	
16	M	147	
17	N	122	
18	O	146	
19	P	144	
20	Q	127	
21	R	118	
22	S	115	
23	T	119	
24	U	102	
25	V	115	
26	W	96	
27	X	103	
28	Y	95	

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Mol	Chain	Length	Quality of chain
29	Z	62	
30	a	1558	
31	c	261	
32	d	218	
33	e	203	
34	f	166	
35	g	100	
36	h	156	
37	i	132	
38	j	130	
39	k	102	
40	l	129	
41	m	137	
42	n	121	
43	o	61	
44	p	89	
45	q	91	
46	r	88	
47	s	79	
48	t	92	
49	u	83	
50	D	77	
51	b	20	
52	F	229	
53	3	89	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 146150 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 ABC-F type ribosomal protection protein Lsa(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	495	Total	C	N	O	S	0	0
			4018	2557	688	764	9		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	142	GLN	GLU	engineered mutation	UNP A0A4U4C430
0	452	GLN	GLU	engineered mutation	UNP A0A4U4C430
0	499	GLY	-	expression tag	UNP A0A4U4C430
0	500	HIS	-	expression tag	UNP A0A4U4C430
0	501	HIS	-	expression tag	UNP A0A4U4C430
0	502	HIS	-	expression tag	UNP A0A4U4C430
0	503	HIS	-	expression tag	UNP A0A4U4C430
0	504	HIS	-	expression tag	UNP A0A4U4C430
0	505	HIS	-	expression tag	UNP A0A4U4C430
0	506	ALA	-	expression tag	UNP A0A4U4C430
0	507	LYS	-	expression tag	UNP A0A4U4C430
0	508	GLY	-	expression tag	UNP A0A4U4C430
0	509	GLY	-	expression tag	UNP A0A4U4C430
0	510	GLU	-	expression tag	UNP A0A4U4C430
0	511	ASN	-	expression tag	UNP A0A4U4C430
0	512	LEU	-	expression tag	UNP A0A4U4C430
0	513	TYR	-	expression tag	UNP A0A4U4C430
0	514	PHE	-	expression tag	UNP A0A4U4C430
0	515	GLN	-	expression tag	UNP A0A4U4C430
0	516	GLY	-	expression tag	UNP A0A4U4C430
0	517	VAL	-	expression tag	UNP A0A4U4C430
0	518	ALA	-	expression tag	UNP A0A4U4C430
0	519	ASP	-	expression tag	UNP A0A4U4C430
0	520	TYR	-	expression tag	UNP A0A4U4C430
0	521	LYS	-	expression tag	UNP A0A4U4C430
0	522	ASP	-	expression tag	UNP A0A4U4C430
0	523	HIS	-	expression tag	UNP A0A4U4C430

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Chain	Residue	Modelled	Actual	Comment	Reference
0	524	ASP	-	expression tag	UNP A0A4U4C430
0	525	GLY	-	expression tag	UNP A0A4U4C430
0	526	ASP	-	expression tag	UNP A0A4U4C430
0	527	TYR	-	expression tag	UNP A0A4U4C430
0	528	LYS	-	expression tag	UNP A0A4U4C430
0	529	ASP	-	expression tag	UNP A0A4U4C430
0	530	HIS	-	expression tag	UNP A0A4U4C430
0	531	ASP	-	expression tag	UNP A0A4U4C430
0	532	ILE	-	expression tag	UNP A0A4U4C430
0	533	ASP	-	expression tag	UNP A0A4U4C430
0	534	TYR	-	expression tag	UNP A0A4U4C430
0	535	LYS	-	expression tag	UNP A0A4U4C430
0	536	ASP	-	expression tag	UNP A0A4U4C430
0	537	ASP	-	expression tag	UNP A0A4U4C430
0	538	ASP	-	expression tag	UNP A0A4U4C430
0	539	ASP	-	expression tag	UNP A0A4U4C430
0	540	LYS	-	expression tag	UNP A0A4U4C430
0	541	GLY	-	expression tag	UNP A0A4U4C430

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			491	307	91	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			428	266	80	81	1		

- Molecule 4 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	53	Total	C	N	O	S	0	0
			406	248	84	69	5		

- Molecule 5 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	48	Total	C	N	O	S	0	0
			410	247	84	75	4		

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	43	Total	C	N	O	S	0	0
			369	224	90	53	2		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			522	320	122	78	2		

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			305	188	66	45	6		

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	2905	Total	C	N	O	P	0	0
			62352	27832	11466	20149	2905		

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	114	Total	C	N	O	P	0	0
			2439	1088	439	798	114		

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	274	Total	C	N	O	S	0	0
			2106	1305	414	380	7		

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	207	Total	C	N	O	S	0	0
			1579	994	292	289	4		

- Molecule 13 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	205	Total	C	N	O	S	0	0
			1572	984	289	297	2		

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	176	Total	C	N	O	S	0	0
			1383	882	237	258	6		

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	174	Total	C	N	O	S	0	0
			1335	838	242	251	4		

- Molecule 16 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	145	Total	C	N	O	S	0	0
			1130	715	205	207	3		

- Molecule 17 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	122	Total	C	N	O	S	0	0
			923	574	176	171	2		

- Molecule 18 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	146	Total	C	N	O	S	0	0
			1096	677	212	206	1		

- Molecule 19 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	134	Total	C	N	O	S	0	0
			1070	683	209	173	5		

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	125	Total	C	N	O	S	0	0
			997	615	192	187	3		

- Molecule 21 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	117	Total	C	N	O	S	0	0
			900	556	175	168	1		

- Molecule 22 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	114	Total	C	N	O	S	0	0
			925	582	185	158			

- Molecule 23 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	116	Total	C	N	O	S	0	0
			935	593	181	157	4		

- Molecule 24 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	101	Total	C	N	O	S	0	0
			779	497	138	142	2		

- Molecule 25 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	111	Total	C	N	O	S	0	0
			841	527	154	158	2		

- Molecule 26 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	91	Total	C	N	O	S	0	0
			736	469	129	134	4		

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	101	Total	C	N	O	S	0	0
			763	486	135	140	2		

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	74	Total	C	N	O		0	0
			559	344	107	108			

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	60	Total	C	N	O	S	0	0
			473	294	96	81	2		

- Molecule 30 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	1517	Total	C	N	O	P	0	0
			32512	14505	5942	10548	1517		

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	222	Total	C	N	O	S	0	0
			1773	1126	312	326	9		

- Molecule 32 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	206	Total	C	N	O	S	0	0
			1626	1024	305	294	3		

- Molecule 33 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	200	Total	C	N	O	S	0	0
			1611	1010	301	296	4		

- Molecule 34 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	163	Total	C	N	O	S	0	0
			1197	752	222	221	2		

- Molecule 35 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	97	Total	C	N	O	S	0	0
			795	501	137	154	3		

- Molecule 36 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	153	Total	C	N	O	S	0	0
			1218	759	232	221	6		

- Molecule 37 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	131	Total	C	N	O	S	0	0
			1041	662	184	193	2		

- Molecule 38 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	128	Total	C	N	O	S	0	0
			989	615	197	176	1		

- Molecule 39 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	96	Total	C	N	O	S	0	0
			773	487	142	142	2		

- Molecule 40 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	116	Total	C	N	O	S	0	0
			854	527	163	160	4		

- Molecule 41 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	135	Total	C	N	O	S	0	0
			1060	658	213	187	2		

- Molecule 42 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	114	Total	C	N	O	S	0	0
			902	552	183	166	1		

- Molecule 43 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	60	Total	C	N	O	S	0	0
			492	310	100	77	5		

- Molecule 44 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	85	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 45 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	87	Total	C	N	O	S	0	0
			692	437	128	125	2		

- Molecule 46 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	81	Total	C	N	O	S	0	0
			669	419	125	122	3		

- Molecule 47 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	66	Total	C	N	O	S	0	0
			542	346	105	90	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	81	Total	C	N	O	S	0	0
			659	424	121	112	2		

- Molecule 49 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	80	Total	C	N	O	S	0	0
			603	368	117	116	2		

- Molecule 50 is a RNA chain called tRNA-fMETi.

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

- Molecule 51 is a RNA chain called RNA (5'-R(P*GP*GP*AP*GP*GP*UP*AP*UP*GP*A P*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
51	b	13	Total	C	N	O	P	0	0
			285	127	57	88	13		

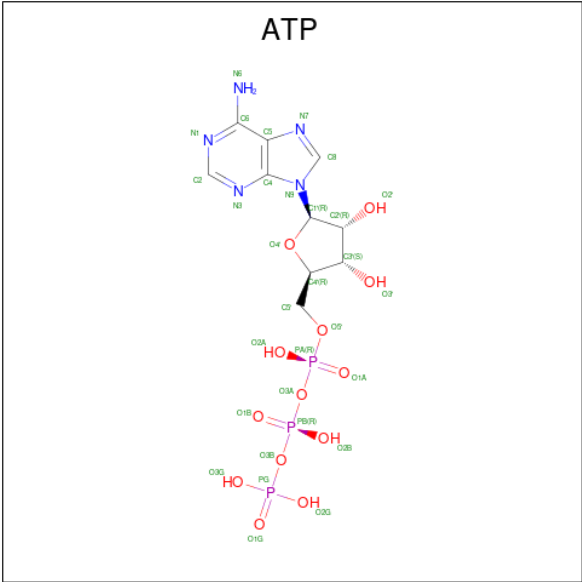
- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	F	132	Total	C	N	O		0	0
			1004	635	172	197			

- Molecule 53 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	55	Total	C	N	O	S	0	0
			448	289	76	81	2		

- Molecule 54 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
54	0	1	Total	C	N	O	P	0
			31	10	5	13	3	
54	0	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	0	2	Total	Mg	0
			2	2	
55	A	117	Total	Mg	0
			117	117	
55	B	1	Total	Mg	0
			1	1	
55	O	1	Total	Mg	0
			1	1	
55	a	25	Total	Mg	0
			25	25	
55	D	1	Total	Mg	0
			1	1	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	4	1	Total	Zn	0
			1	1	

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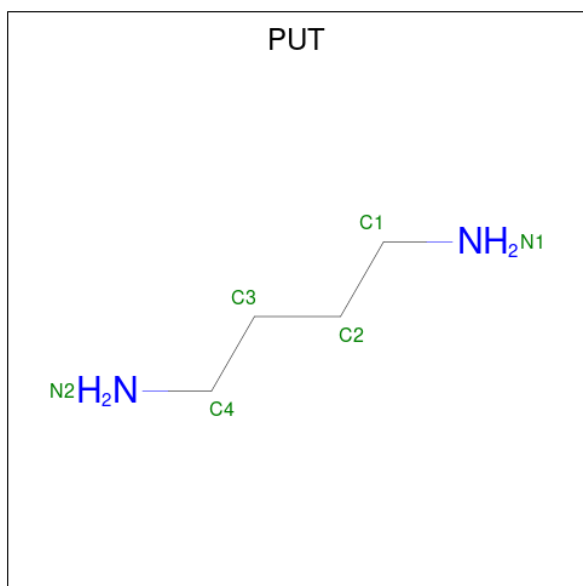
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Mol	Chain	Residues	Atoms		AltConf
56	8	1	Total	Zn	0
			1	1	
56	o	1	Total	Zn	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
57	A	21	Total	K	0
			21	21	
57	P	1	Total	K	0
			1	1	
57	a	7	Total	K	0
			7	7	

- Molecule 58 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).

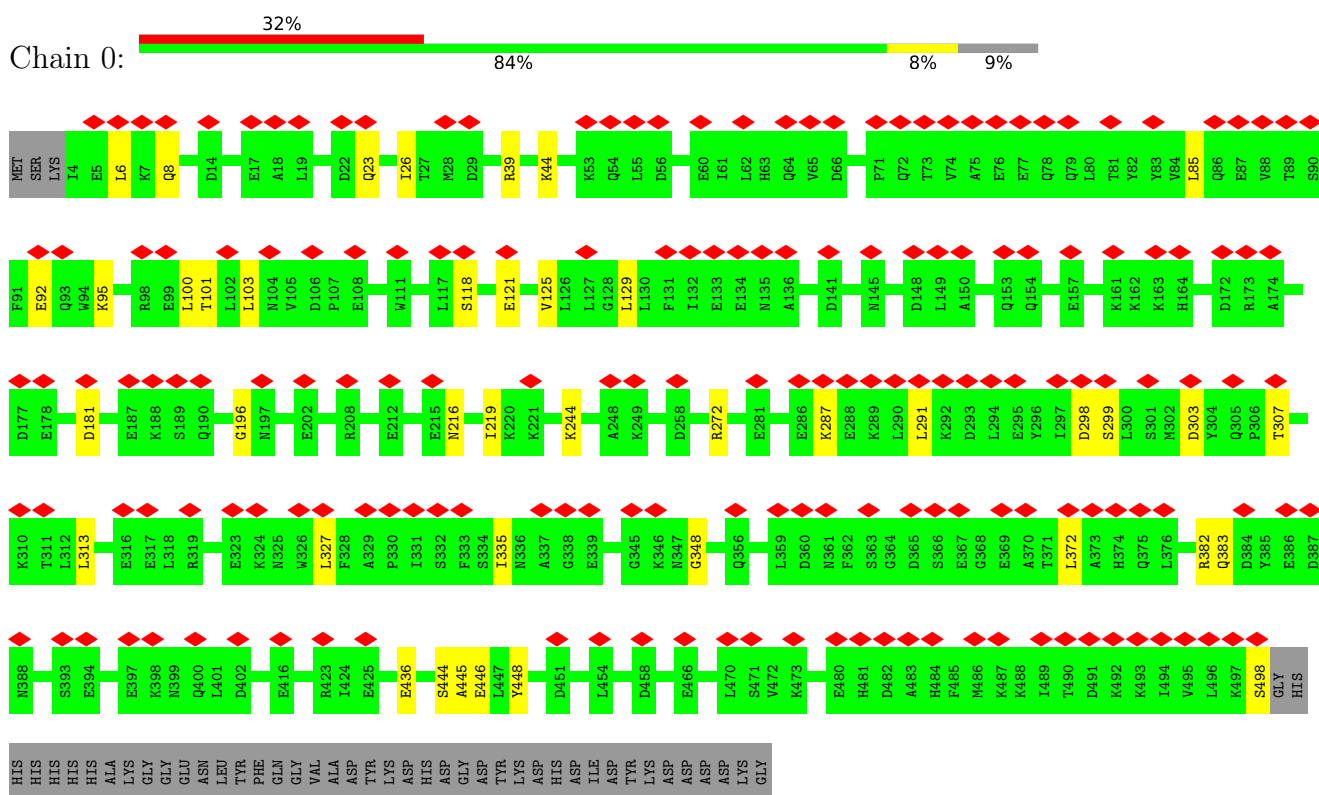


Mol	Chain	Residues	Atoms			AltConf
58	A	1	Total	C	N	0
			6	4	2	
58	A	1	Total	C	N	0
			6	4	2	
58	a	1	Total	C	N	0
			6	4	2	
58	a	1	Total	C	N	0
			6	4	2	

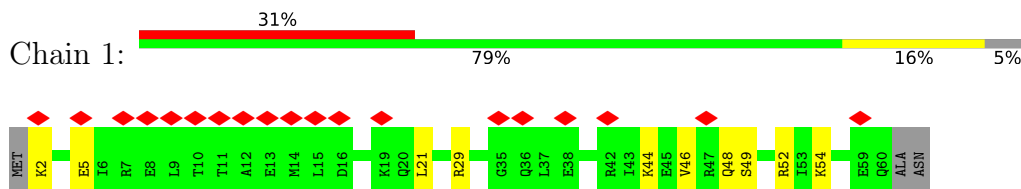
3 Residue-property plots

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

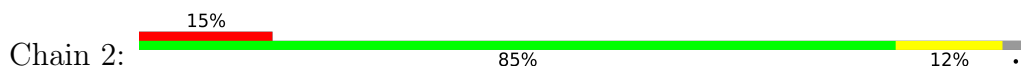
- Molecule 1: ABC-F type ribosomal protection protein Lsa(A)

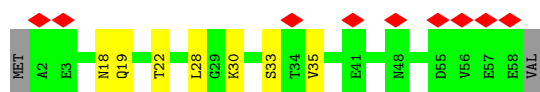


- Molecule 2: 50S ribosomal protein L29

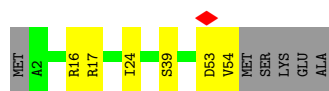
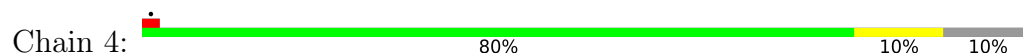


- Molecule 3: 50S ribosomal protein L30

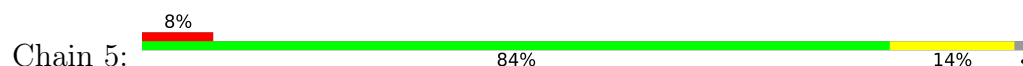




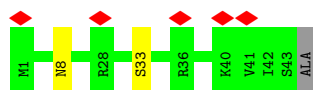
- Molecule 4: 50S ribosomal protein L32



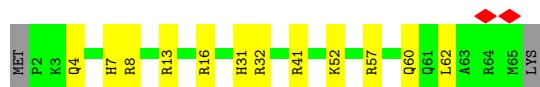
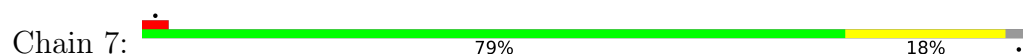
- Molecule 5: 50S ribosomal protein L33



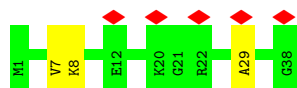
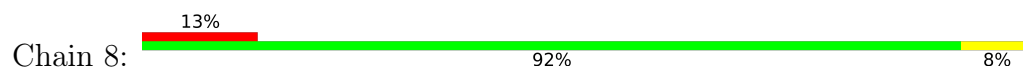
- Molecule 6: 50S ribosomal protein L34



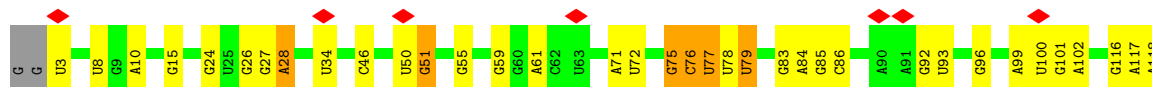
- Molecule 7: 50S ribosomal protein L35

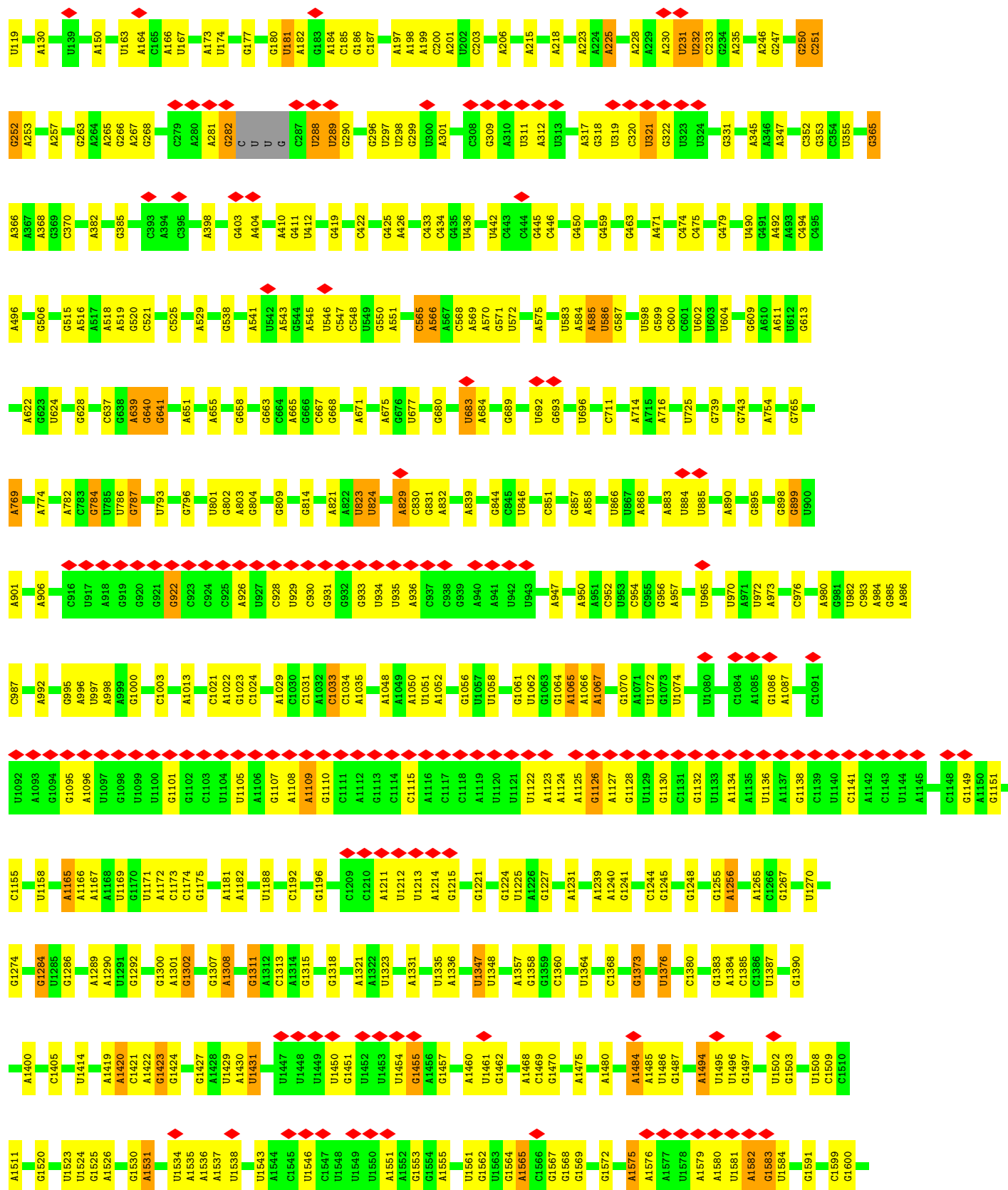


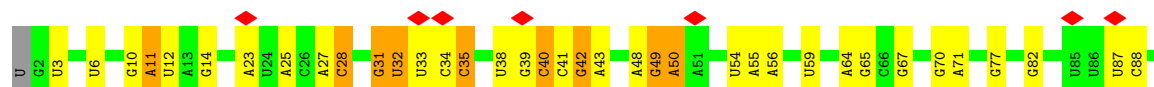
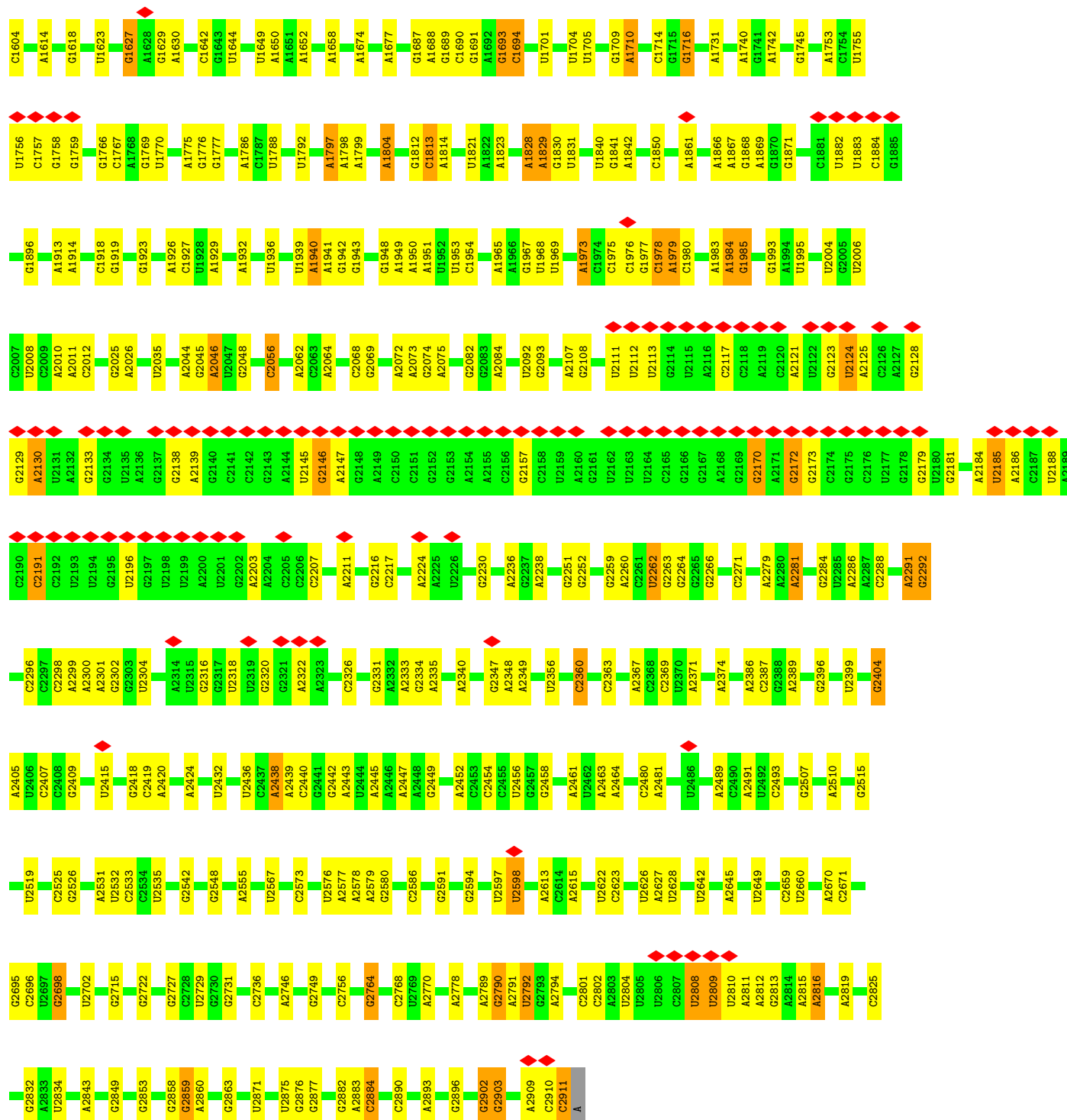
- Molecule 8: 50S ribosomal protein L36

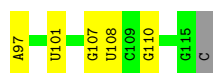


- Molecule 9: 23S rRNA



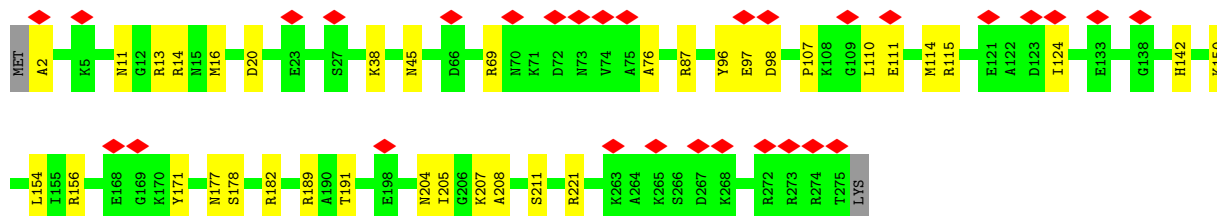






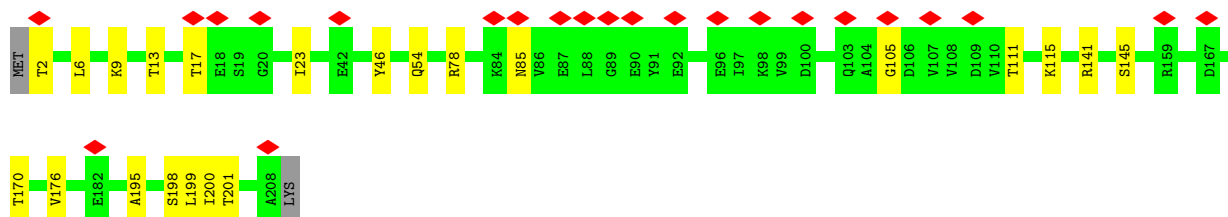
- Molecule 11: 50S ribosomal protein L2

Chain G: 11% 86% 13% .



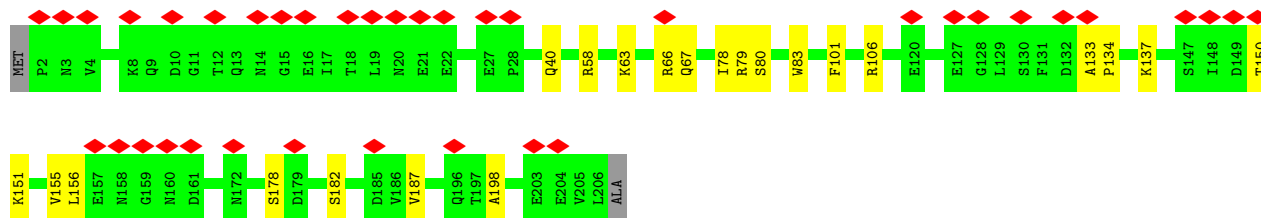
- Molecule 12: 50S ribosomal protein L3

Chain H: 11% 89% 11% .



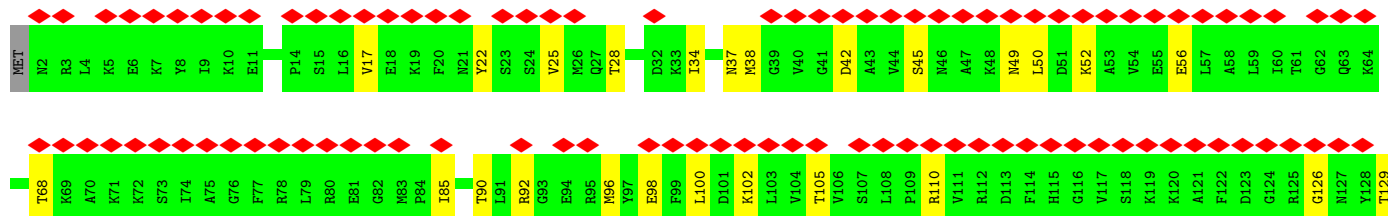
- Molecule 13: 50S ribosomal protein L4

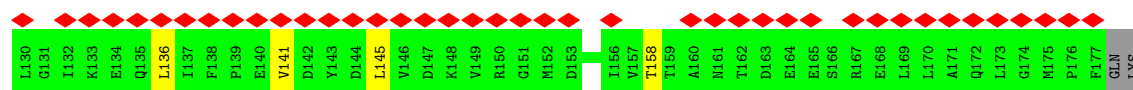
Chain I: 18% 88% 11% .



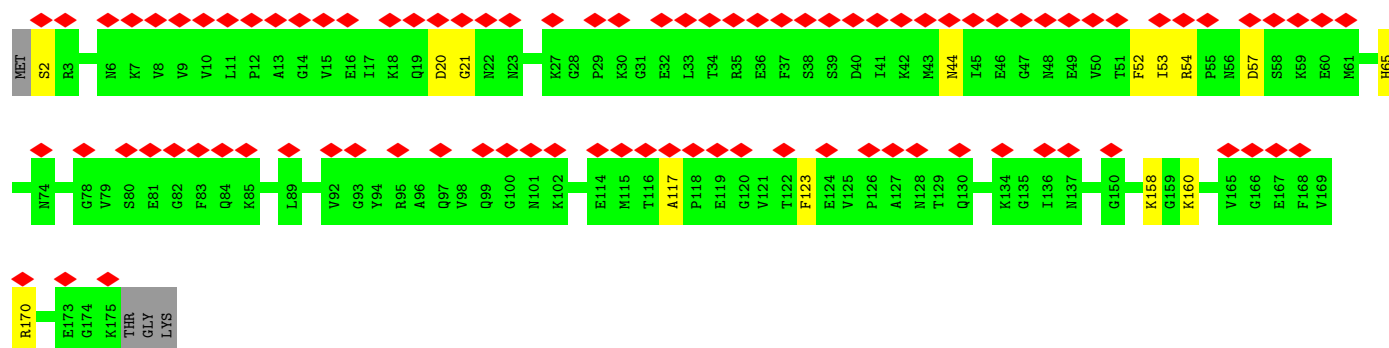
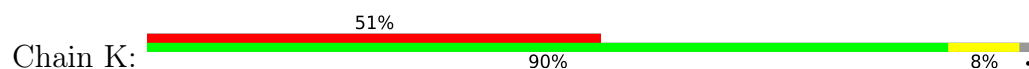
- Molecule 14: 50S ribosomal protein L5

Chain J: 77% 82% 16% .

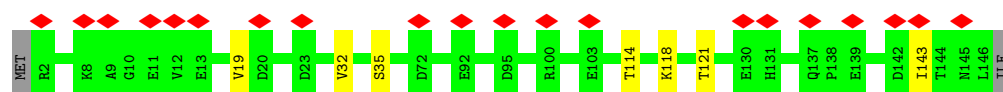




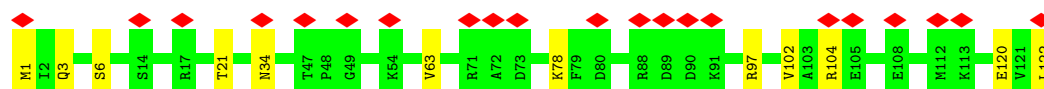
- Molecule 15: 50S ribosomal protein L6



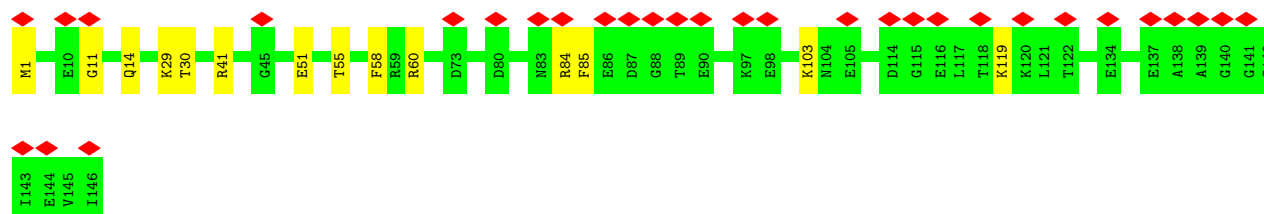
- Molecule 16: 50S ribosomal protein L13



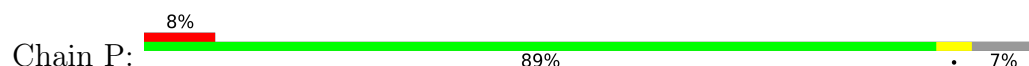
- Molecule 17: 50S ribosomal protein L14

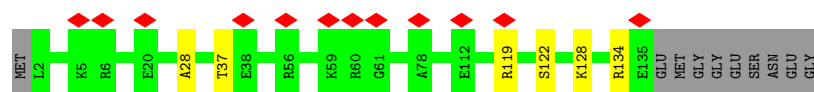


- Molecule 18: 50S ribosomal protein L15

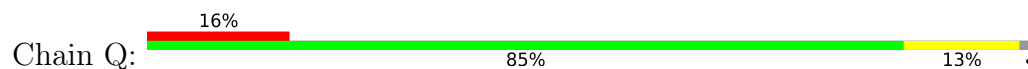


- Molecule 19: 50S ribosomal protein L16

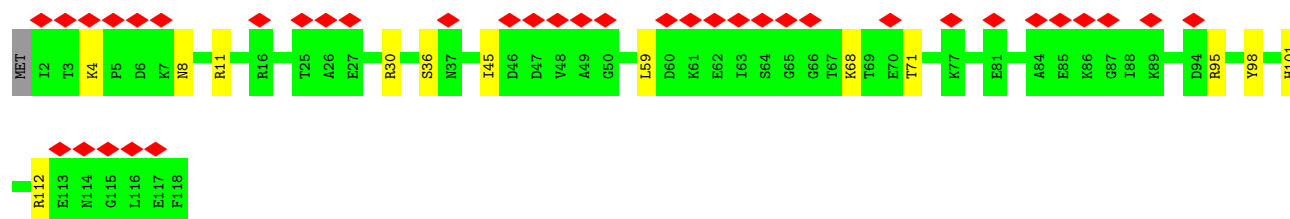
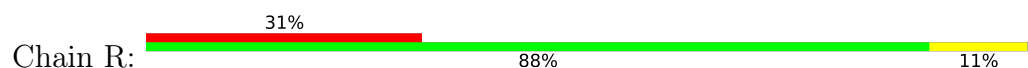




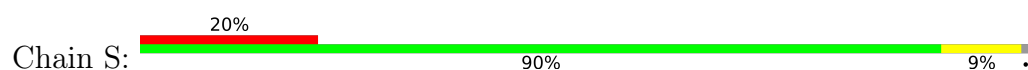
- Molecule 20: 50S ribosomal protein L17



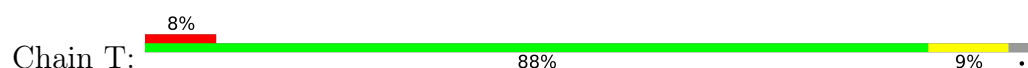
- Molecule 21: 50S ribosomal protein L18



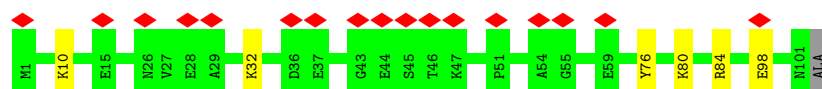
- Molecule 22: 50S ribosomal protein L19



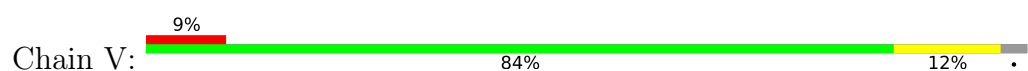
- Molecule 23: 50S ribosomal protein L20

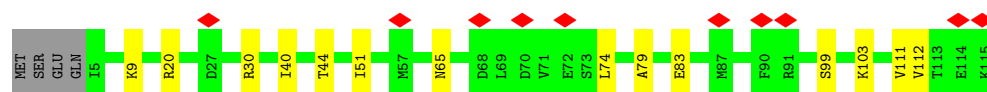


- Molecule 24: 50S ribosomal protein L21

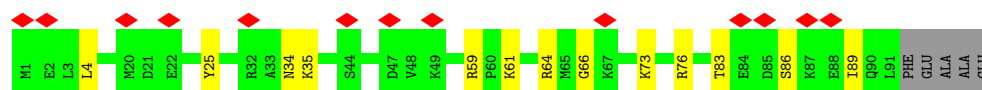
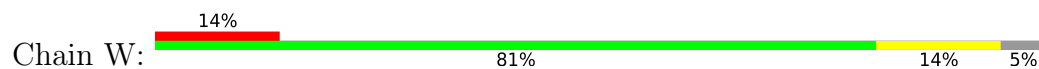


- Molecule 25: 50S ribosomal protein L22

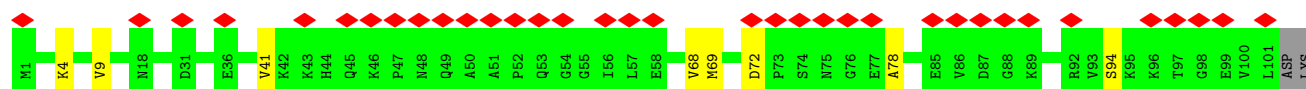
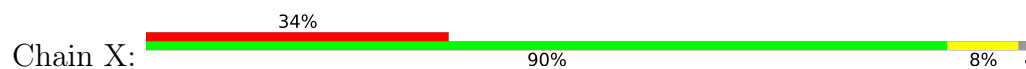




- Molecule 26: 50S ribosomal protein L23



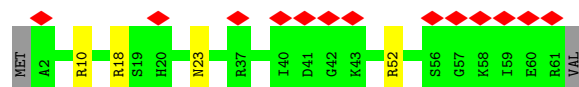
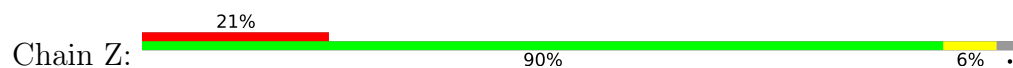
- Molecule 27: 50S ribosomal protein L24



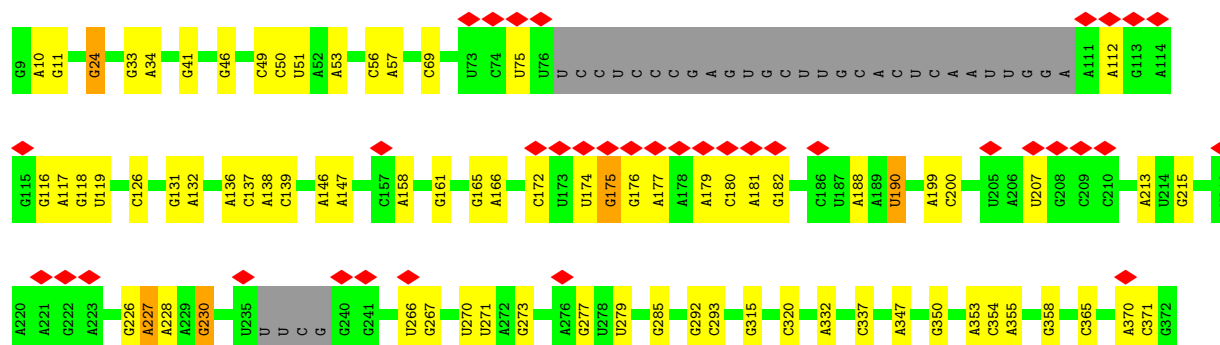
- Molecule 28: 50S ribosomal protein L27

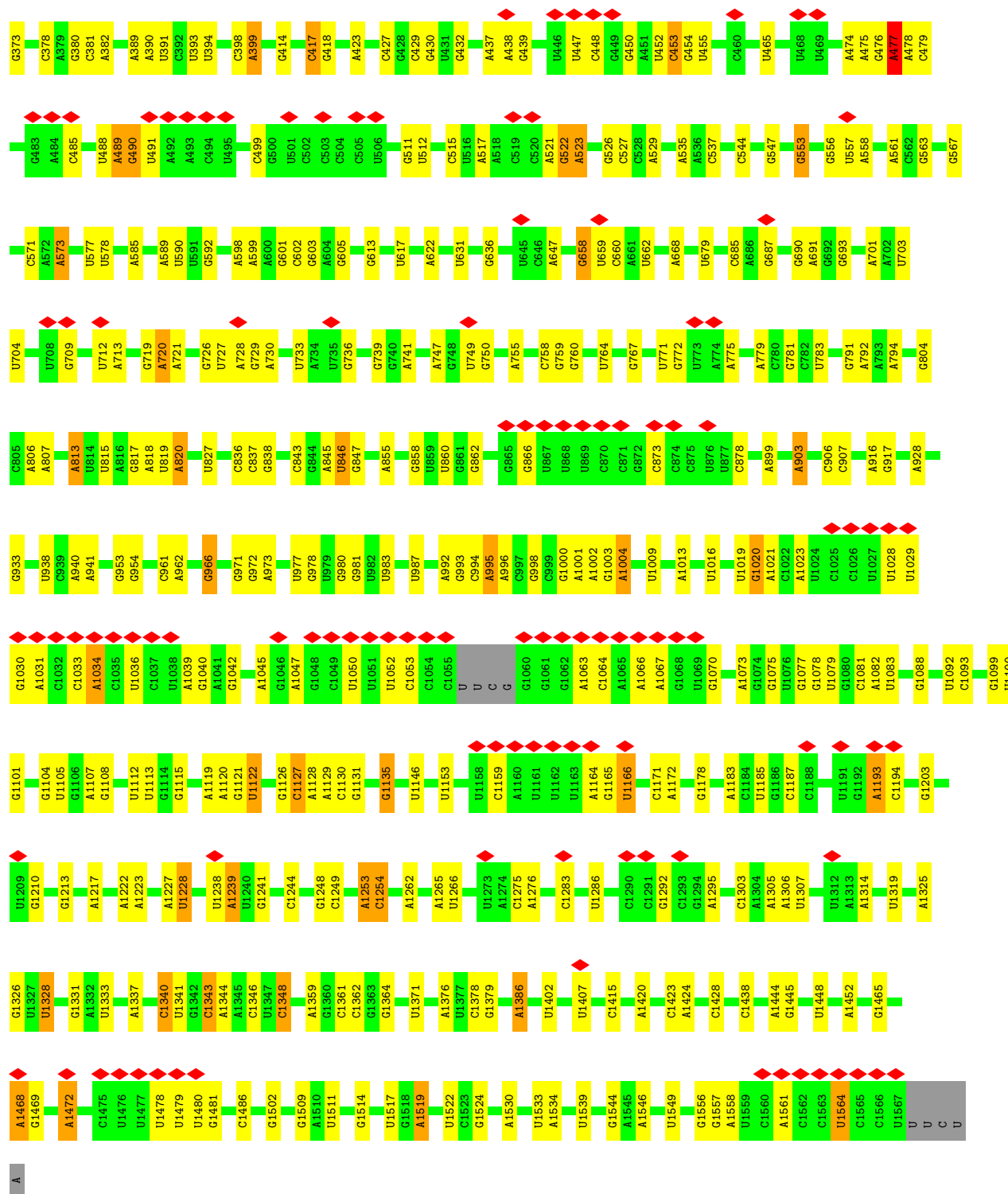


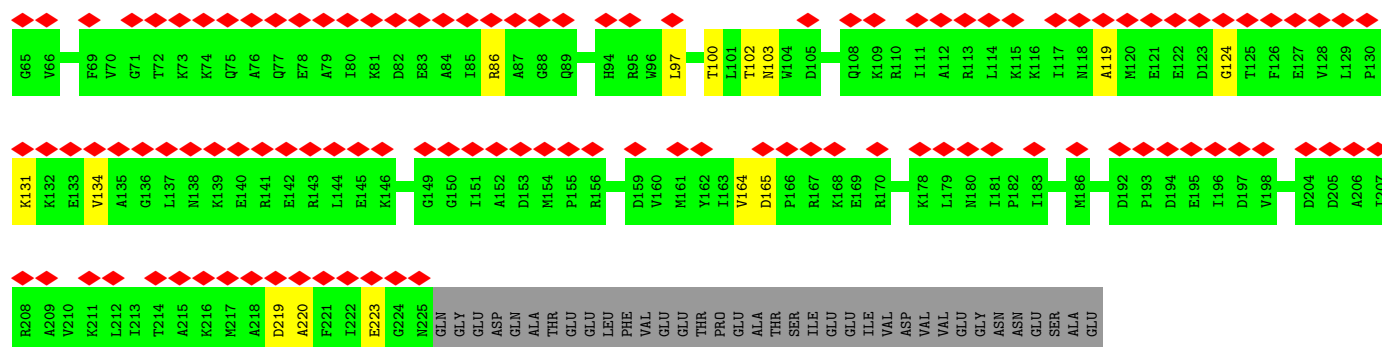
- Molecule 29: 50S ribosomal protein L28



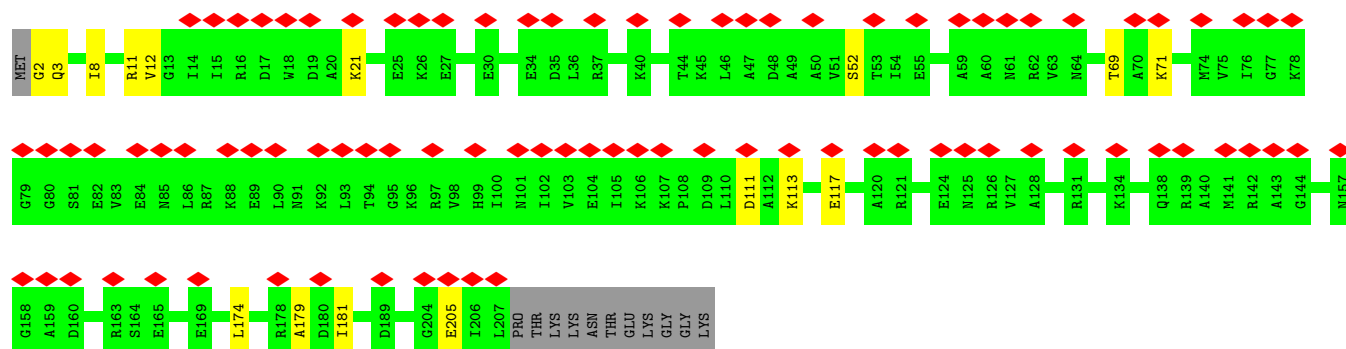
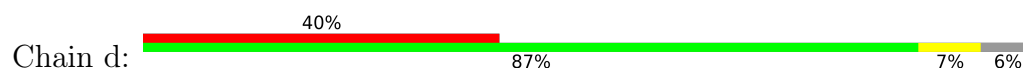
- Molecule 30: 16S rRNA



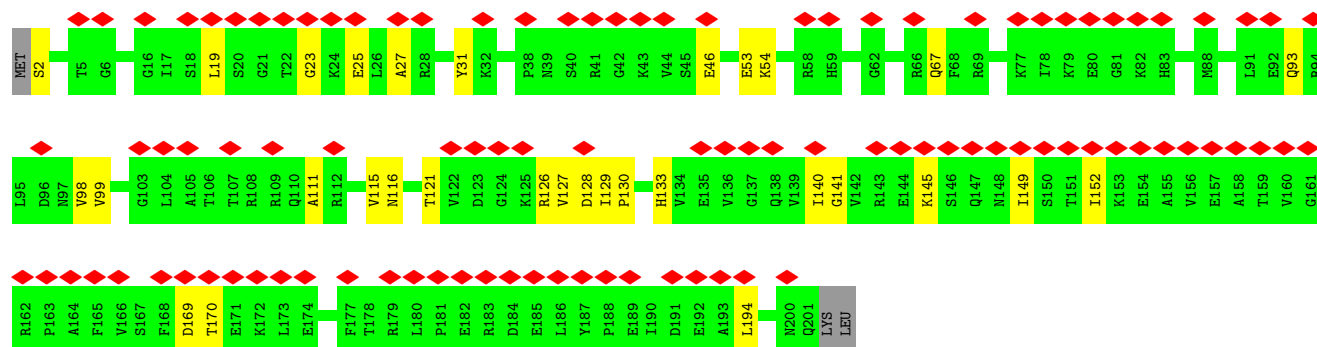
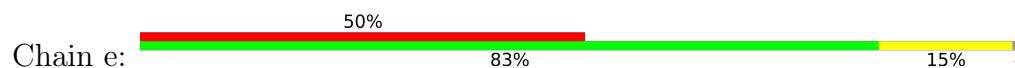




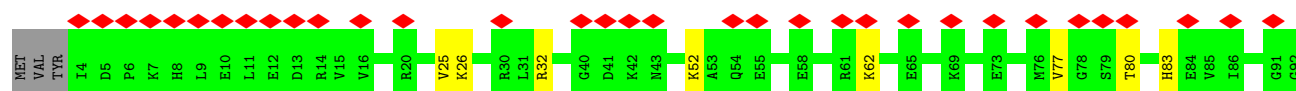
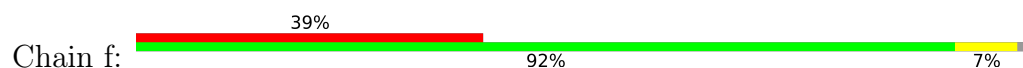
• Molecule 32: 30S ribosomal protein S3

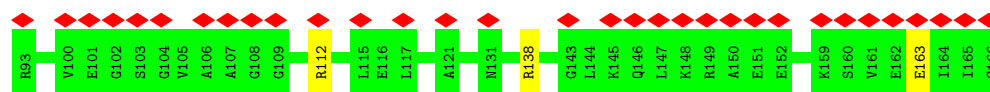


• Molecule 33: 30S ribosomal protein S4

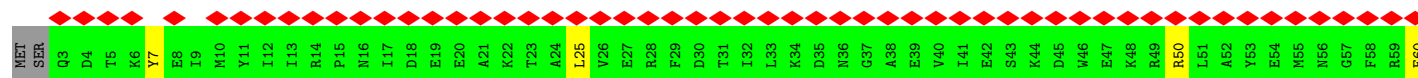
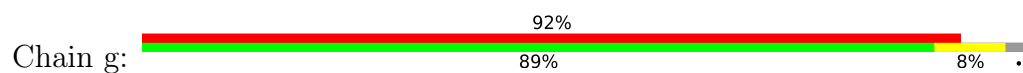


• Molecule 34: 30S ribosomal protein S5

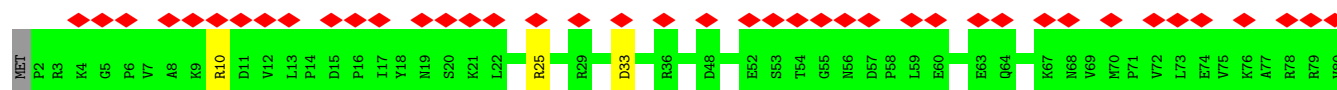




- Molecule 35: 30S ribosomal protein S6



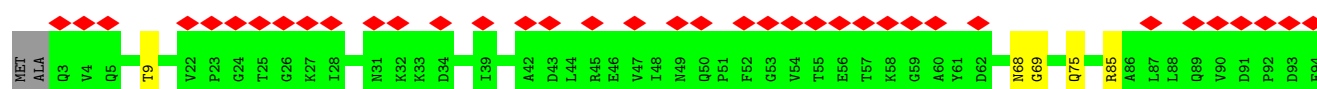
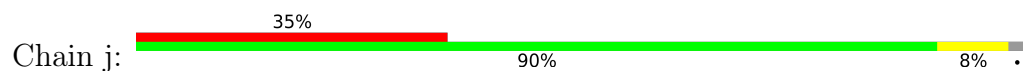
- Molecule 36: 30S ribosomal protein S7



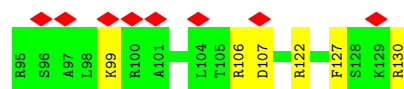
- Molecule 37: 30S ribosomal protein S8

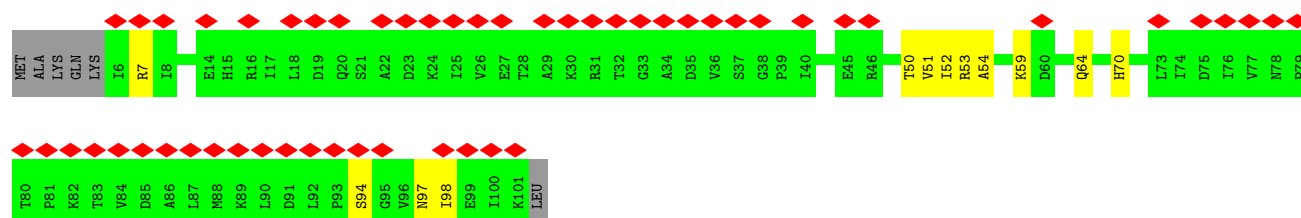
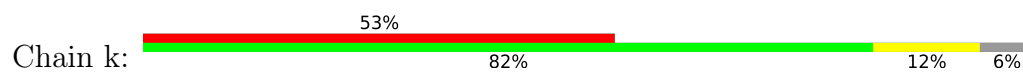


- Molecule 38: 30S ribosomal protein S9

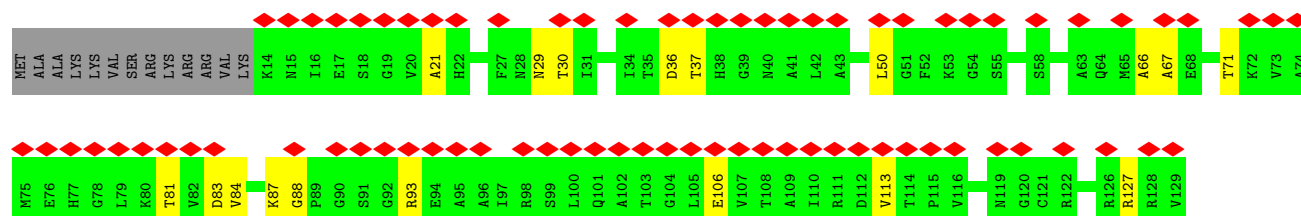
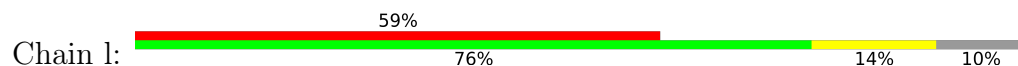


- Molecule 39: 30S ribosomal protein S10

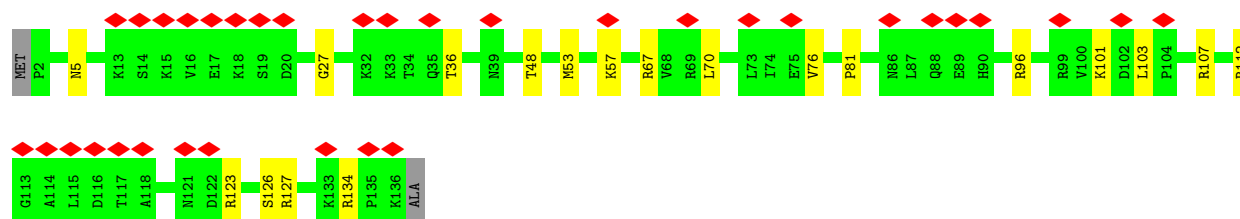
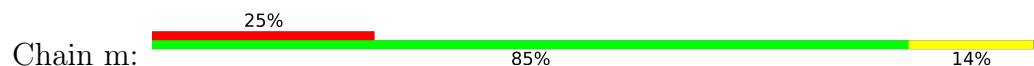




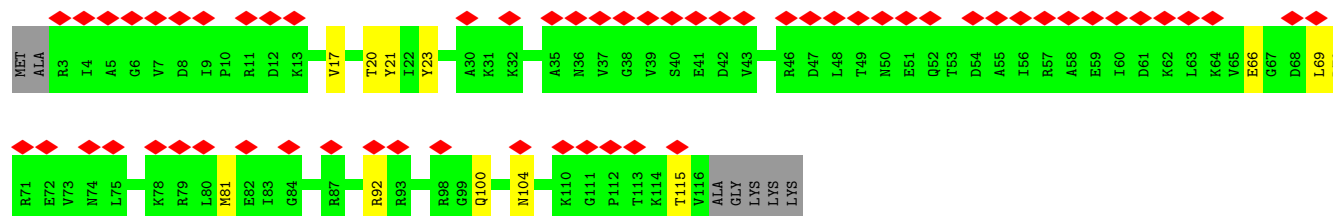
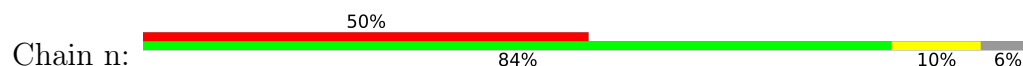
- Molecule 40: 30S ribosomal protein S11



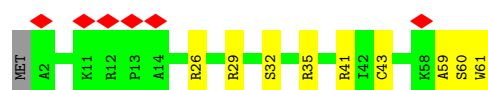
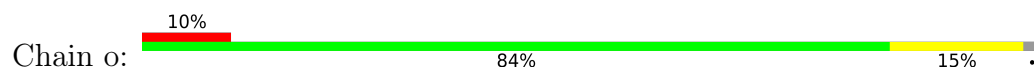
- Molecule 41: 30S ribosomal protein S12



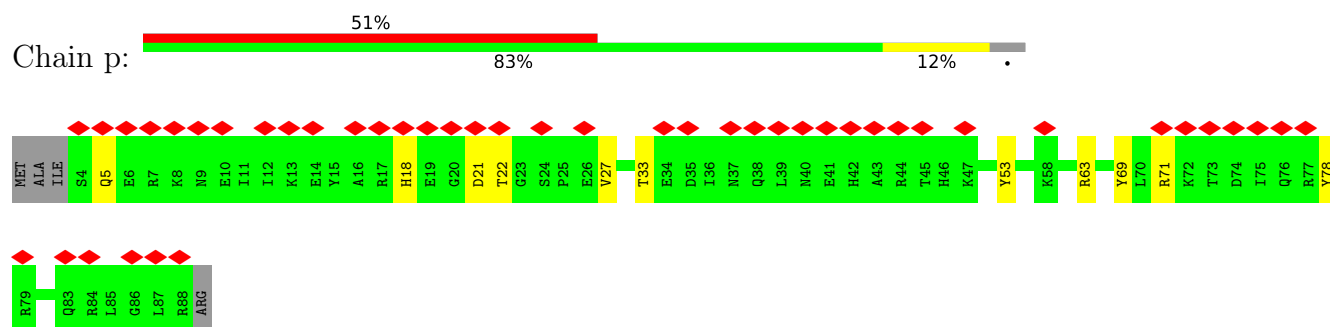
- Molecule 42: 30S ribosomal protein S13



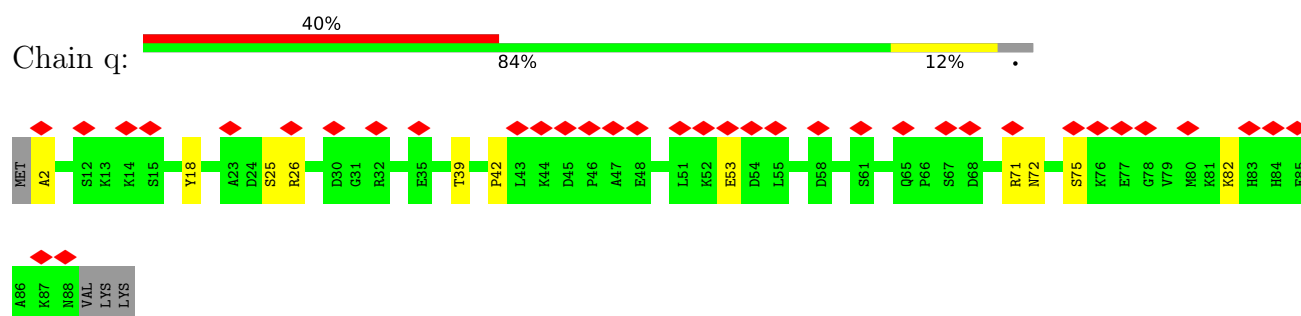
- Molecule 43: 30S ribosomal protein S14 type Z



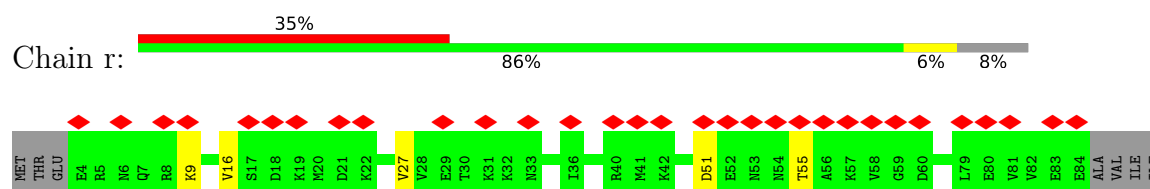
- Molecule 44: 30S ribosomal protein S15



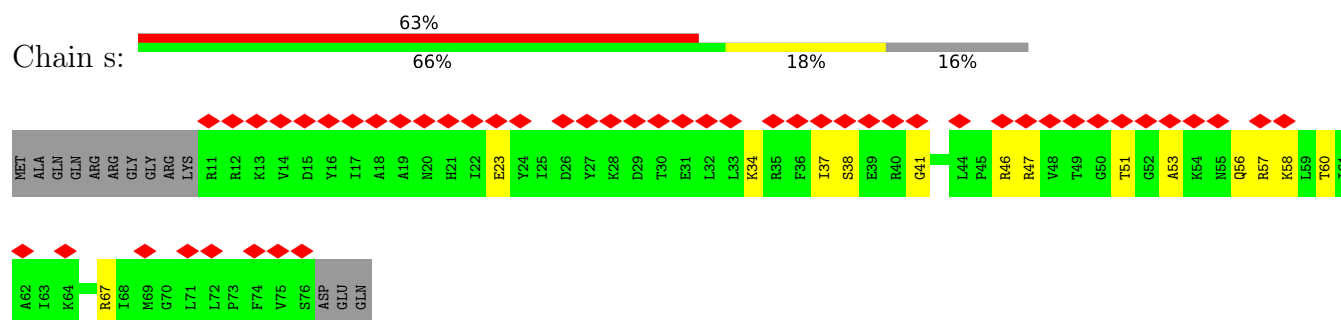
- Molecule 45: 30S ribosomal protein S16



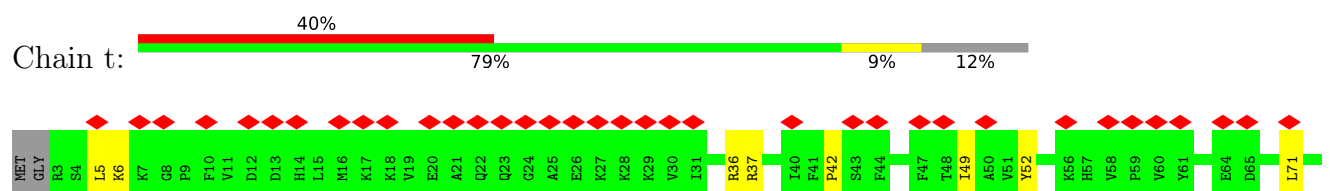
- Molecule 46: 30S ribosomal protein S17

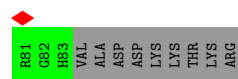


- Molecule 47: 30S ribosomal protein S18

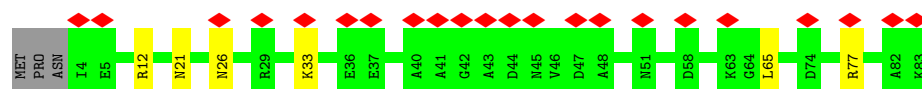
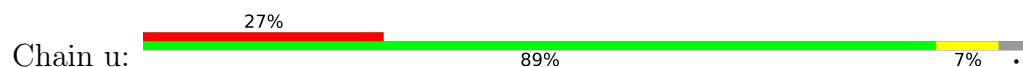


- Molecule 48: 30S ribosomal protein S19

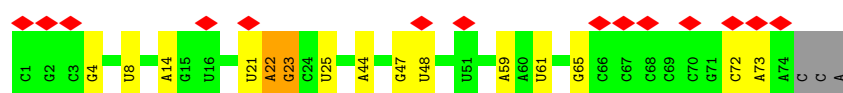
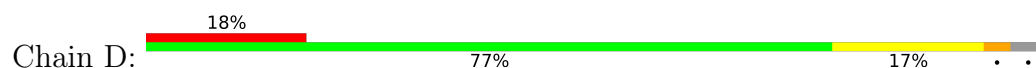




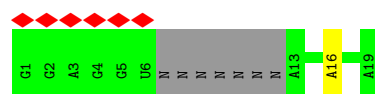
- Molecule 49: 30S ribosomal protein S20



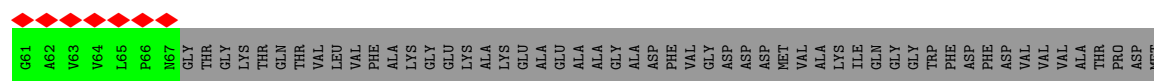
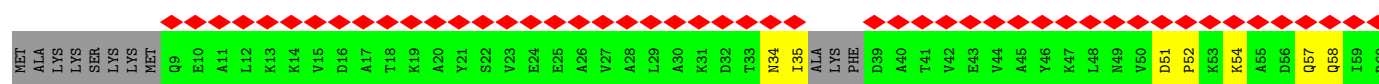
- Molecule 50: tRNA-fMETi



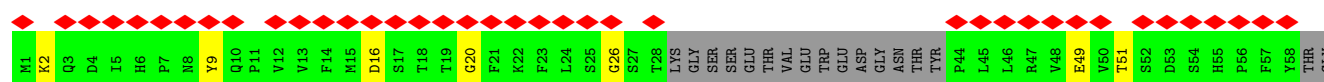
- Molecule 51: RNA (5'-R(P*GP*GP*AP*GP*GP*UP*AP*UP*GP*AP*CP*AP*A)-3')



- Molecule 52: 50S ribosomal protein L1



- Molecule 53: 50S ribosomal protein L31 type B



ARG	GLN	LYS	PHE	THR	GLN	ALA	ASP	G69	R70	V71	D72	R73	F74	N75	K76	K77	Y78	G79	L80	LYS	ASP	GLU	ASN	ALA	ASN	PRO	ASP	ALA
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59262	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 ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	366.432, 366.432, 366.432	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, K, PUT, MG

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	0.30	0/4089	0.44	0/5506
2	1	0.29	0/492	0.48	0/654
3	2	0.33	0/430	0.48	0/579
4	4	0.42	0/413	0.50	0/549
5	5	0.37	0/414	0.53	0/552
6	6	0.42	0/372	0.51	0/484
7	7	0.44	0/528	0.54	0/689
8	8	0.39	0/310	0.39	0/409
9	A	0.34	0/69847	0.40	1/108953 (0.0%)
10	B	0.24	0/2728	0.35	0/4252
11	G	0.42	0/2141	0.51	0/2881
12	H	0.44	0/1601	0.48	0/2150
13	I	0.41	0/1595	0.48	0/2157
14	J	0.26	0/1402	0.47	0/1885
15	K	0.25	0/1355	0.41	0/1825
16	M	0.44	0/1151	0.53	0/1555
17	N	0.40	0/930	0.46	0/1247
18	O	0.40	0/1106	0.48	0/1474
19	P	0.38	0/1093	0.46	0/1457
20	Q	0.38	0/1006	0.49	0/1349
21	R	0.31	0/909	0.46	0/1216
22	S	0.38	0/939	0.49	0/1262
23	T	0.45	0/948	0.52	0/1261
24	U	0.38	0/791	0.44	0/1061
25	V	0.42	0/850	0.46	0/1145
26	W	0.41	0/743	0.50	0/993
27	X	0.30	0/772	0.45	0/1035
28	Y	0.41	0/565	0.44	0/755
29	Z	0.36	0/479	0.50	0/638
30	a	0.27	0/36394	0.38	2/56758 (0.0%)
31	c	0.23	0/1803	0.43	0/2430
32	d	0.31	0/1651	0.41	0/2219

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.28	0/1641	0.46	0/2206
34	f	0.30	0/1209	0.43	0/1628
35	g	0.22	0/807	0.41	0/1087
36	h	0.31	0/1238	0.45	0/1668
37	i	0.28	0/1054	0.51	0/1417
38	j	0.34	0/1002	0.53	0/1343
39	k	0.30	0/785	0.49	0/1059
40	l	0.35	0/869	0.50	0/1174
41	m	0.36	0/1077	0.48	0/1446
42	n	0.26	0/908	0.45	0/1219
43	o	0.35	0/504	0.54	0/669
44	p	0.26	0/726	0.43	0/969
45	q	0.30	0/704	0.48	0/945
46	r	0.28	0/677	0.44	0/903
47	s	0.24	0/549	0.42	0/733
48	t	0.24	0/676	0.41	0/906
49	u	0.28	0/605	0.41	0/807
50	D	0.28	0/1768	0.39	0/2755
51	b	0.23	0/319	0.38	0/494
52	F	0.19	0/1015	0.42	0/1373
53	3	0.27	0/459	0.45	0/615
All	All	0.32	0/158439	0.41	3/236796 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2438	A	C4'-C3'-O3'	6.87	119.70	109.40
30	a	131	G	C2'-C3'-O3'	6.27	118.90	109.50
30	a	477	A	C4'-C3'-O3'	6.20	118.70	109.40

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	4018	0	4031	29	0
2	1	491	0	527	7	0
3	2	428	0	463	5	0
4	4	406	0	417	5	0
5	5	410	0	425	6	0
6	6	369	0	419	2	0
7	7	522	0	576	11	0
8	8	305	0	337	3	0
9	A	62352	0	31331	252	0
10	B	2439	0	1228	18	0
11	G	2106	0	2189	24	0
12	H	1579	0	1661	14	0
13	I	1572	0	1614	14	0
14	J	1383	0	1446	21	0
15	K	1335	0	1369	9	0
16	M	1130	0	1168	8	0
17	N	923	0	985	9	0
18	O	1096	0	1149	11	0
19	P	1070	0	1136	3	0
20	Q	997	0	1033	13	0
21	R	900	0	932	10	0
22	S	925	0	979	10	0
23	T	935	0	991	10	0
24	U	779	0	821	5	0
25	V	841	0	898	12	0
26	W	736	0	795	11	0
27	X	763	0	824	5	0
28	Y	559	0	568	9	0
29	Z	473	0	513	4	0
30	a	32512	0	16377	152	0
31	c	1773	0	1810	14	0
32	d	1626	0	1675	10	0
33	e	1611	0	1628	20	0
34	f	1197	0	1274	12	0
35	g	795	0	789	5	0
36	h	1218	0	1246	6	0
37	i	1041	0	1092	26	0
38	j	989	0	1035	9	0
39	k	773	0	814	9	0
40	l	854	0	869	11	0
41	m	1060	0	1128	15	0
42	n	902	0	956	10	0
43	o	492	0	509	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	p	716	0	727	7	0
45	q	692	0	724	7	0
46	r	669	0	705	3	0
47	s	542	0	588	9	0
48	t	659	0	672	8	0
49	u	603	0	634	5	0
50	D	1582	0	802	4	0
51	b	285	0	143	0	0
52	F	1004	0	1032	10	0
53	3	448	0	439	10	0
54	0	62	0	24	6	0
55	0	2	0	0	0	0
55	A	117	0	0	0	0
55	B	1	0	0	0	0
55	D	1	0	0	0	0
55	O	1	0	0	0	0
55	a	25	0	0	0	0
56	4	1	0	0	0	0
56	8	1	0	0	0	0
56	o	1	0	0	0	0
57	A	21	0	0	0	0
57	P	1	0	0	0	0
57	a	7	0	0	0	0
58	A	12	0	24	0	0
58	a	12	0	24	0	0
All	All	146150	0	98565	699	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 (699) 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)
30:a:631:U:N3	30:a:658:G:O6	2.05	0.88
9:A:1831:U:O2'	11:G:154:LEU:O	1.95	0.83
12:H:111:THR:HG1	12:H:201:THR:HG1	1.13	0.82
1:0:348:GLY:HA2	54:0:601:ATP:H5'2	1.61	0.81
9:A:2671:C:OP1	15:K:158:LYS:NZ	2.14	0.80
16:M:32:VAL:HG21	16:M:143:ILE:HD12	1.63	0.79
7:7:32:ARG:NH1	9:A:2404:G:OP2	2.16	0.79
9:A:2191:C:O2'	52:F:170:ASN:OD1	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:38:U:O2'	10:B:43:A:N6	2.16	0.78
18:O:55:THR:O	18:O:60:ARG:NH2	2.17	0.78
23:T:48:ARG:NH1	23:T:49:ASP:OD1	2.17	0.77
44:p:71:ARG:NH2	44:p:78:TYR:OH	2.18	0.77
9:A:637:C:O2'	9:A:641:G:OP1	2.03	0.76
9:A:2128:G:O2'	9:A:2179:G:N2	2.18	0.76
9:A:1828:A:O2'	9:A:1829:A:O5'	2.01	0.76
14:J:105:THR:O	53:3:51:THR:OG1	2.03	0.76
9:A:319:U:O2'	9:A:321:U:OP2	2.04	0.76
30:a:517:A:OP1	33:e:145:LYS:NZ	2.19	0.75
30:a:571:C:OP1	33:e:54:LYS:NZ	2.19	0.75
1:0:118:SER:OG	1:0:121:GLU:OE1	2.02	0.75
9:A:986:A:O2'	9:A:1023:G:N2	2.19	0.75
30:a:792:A:OP2	30:a:838:G:N2	2.19	0.75
30:a:452:U:OP1	33:e:31:TYR:OH	2.03	0.75
52:F:215:THR:OG1	52:F:219:GLY:O	2.03	0.75
30:a:1013:A:N3	48:t:52:TYR:OH	2.20	0.74
30:a:577:U:O2'	41:m:96:ARG:NH2	2.19	0.74
30:a:713:A:O2'	30:a:727:U:O4	2.05	0.74
9:A:899:G:O2'	9:A:956:G:O6	2.05	0.74
2:1:54:LYS:NZ	9:A:72:U:OP2	2.21	0.74
9:A:368:A:O2'	9:A:370:C:OP2	2.05	0.74
14:J:68:THR:OG1	14:J:85:ILE:O	2.07	0.73
9:A:436:U:OP2	29:Z:10:ARG:NH1	2.21	0.73
9:A:1993:G:O2'	9:A:1995:U:OP2	2.06	0.73
9:A:1284:G:OP1	23:T:2:ALA:N	2.22	0.73
9:A:1564:G:OP2	9:A:1565:A:O2'	2.06	0.73
30:a:1346:C:N3	48:t:36:ARG:NH1	2.36	0.73
9:A:2026:A:HO2'	25:V:99:SER:HG	1.16	0.73
9:A:639:A:N1	9:A:663:G:O2'	2.20	0.72
35:g:81:ASP:OD2	35:g:85:LYS:NZ	2.22	0.72
9:A:2092:U:O2'	29:Z:23:ASN:OD1	2.07	0.72
9:A:2271:C:O2'	9:A:2440:C:OP2	2.06	0.72
1:0:8:GLN:NE2	1:0:23:GLN:OE1	2.23	0.72
9:A:640:G:OP1	18:O:84:ARG:NH2	2.22	0.72
9:A:1067:A:OP2	9:A:1165:A:N6	2.23	0.72
12:H:111:THR:HG22	12:H:170:THR:HG22	1.71	0.72
38:j:106:ARG:NH1	38:j:107:ASP:O	2.23	0.72
4:4:24:ILE:HD11	25:V:44:THR:HG23	1.72	0.71
30:a:399:A:N1	30:a:417:C:O2'	2.23	0.71
30:a:613:G:OP1	37:i:86:ARG:NH2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:D:59:A:O2'	50:D:61:U:OP2	2.05	0.71
20:Q:18:ARG:NE	20:Q:65:PHE:O	2.23	0.71
11:G:69:ARG:O	11:G:189:ARG:NH1	2.23	0.71
14:J:42:ASP:OD1	14:J:45:SER:OG	2.09	0.71
30:a:764:U:OP1	35:g:7:TYR:OH	2.06	0.71
9:A:1373:G:N7	26:W:61:LYS:NZ	2.39	0.70
32:d:52:SER:OG	32:d:111:ASP:OD2	2.04	0.70
5:5:4:ASN:ND2	5:5:20:ASN:OD1	2.24	0.70
9:A:1311:G:OP2	9:A:1687:G:O2'	2.08	0.70
10:B:6:U:OP1	21:R:11:ARG:NH1	2.24	0.70
37:i:79:ARG:NE	37:i:81:SER:O	2.25	0.70
30:a:126:C:O2'	45:q:26:ARG:O	2.08	0.70
7:7:13:ARG:NH2	9:A:252:G:OP1	2.25	0.70
37:i:5:ASP:OD1	37:i:79:ARG:NH1	2.24	0.70
9:A:2056:C:OP1	9:A:2790:G:O2'	2.08	0.70
9:A:2263:G:OP1	9:A:2288:C:O2'	2.09	0.70
9:A:1487:G:O6	9:A:1508:U:O2	2.10	0.70
9:A:2832:G:O2'	9:A:2834:U:OP2	2.07	0.70
9:A:1029:A:O2'	9:A:1031:C:OP2	2.09	0.70
19:P:28:ALA:O	19:P:134:ARG:NH1	2.23	0.70
5:5:2:ARG:NH2	9:A:2298:C:OP2	2.25	0.69
8:8:8:LYS:NZ	9:A:2480:C:OP1	2.24	0.69
13:I:58:ARG:O	13:I:79:ARG:NH1	2.25	0.69
30:a:1213:G:N3	43:o:60:SER:OG	2.25	0.69
30:a:617:U:OP1	37:i:31:LYS:NZ	2.26	0.69
30:a:779:A:OP1	44:p:69:TYR:OH	2.11	0.69
9:A:355:U:OP2	13:I:137:LYS:NZ	2.25	0.69
9:A:76:C:O2'	9:A:77:U:OP2	2.09	0.69
30:a:499:C:OP2	45:q:71:ARG:NH2	2.25	0.69
26:W:64:ARG:NH2	26:W:66:GLY:O	2.25	0.69
16:M:118:LYS:O	16:M:121:THR:OG1	2.10	0.68
9:A:2146:G:N2	9:A:2170:G:O2'	2.26	0.68
30:a:1465:G:OP1	49:u:33:LYS:NZ	2.26	0.68
30:a:515:C:OP1	33:e:126:ARG:NH2	2.26	0.68
9:A:1423:G:O2'	9:A:1568:G:O2'	2.11	0.68
31:c:54:TYR:OH	31:c:223:GLU:OE1	2.12	0.68
33:e:19:LEU:N	33:e:25:GLU:OE2	2.26	0.68
17:N:3:GLN:O	17:N:21:THR:OG1	2.08	0.67
9:A:2356:U:O2'	9:A:2386:A:O2'	2.12	0.67
9:A:1313:C:H4'	20:Q:30:ILE:HD11	1.77	0.67
9:A:1048:A:N3	9:A:1192:C:O2'	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1438:C:OP1	41:m:67:ARG:NH1	2.27	0.67
9:A:2124:U:O4	9:A:2157:G:O2'	2.11	0.67
17:N:1:MET:N	17:N:34:ASN:OD1	2.28	0.67
30:a:1333:U:OP1	42:n:100:GLN:NE2	2.27	0.67
9:A:296:G:N2	9:A:297:U:O4	2.28	0.67
9:A:898:G:O2'	9:A:2281:A:O2'	2.06	0.67
7:7:4:GLN:NE2	7:7:60:GLN:OE1	2.28	0.67
9:A:868:A:N7	9:A:2260:A:O2'	2.28	0.67
30:a:807:A:O2'	30:a:1549:U:O2	2.12	0.67
42:n:17:VAL:O	42:n:20:THR:OG1	2.12	0.66
2:1:2:LYS:N	2:1:5:GLU:OE2	2.28	0.66
9:A:784:G:O2'	9:A:787:G:O2'	2.10	0.66
9:A:2326:C:O4'	14:J:37:ASN:ND2	2.28	0.66
9:A:2389:A:N3	21:R:112:ARG:NH2	2.44	0.66
1:0:303:ASP:OD2	1:0:444:SER:OG	2.09	0.66
30:a:563:G:OP1	41:m:123:ARG:NH2	2.28	0.66
1:0:272:ARG:NH2	9:A:2449:G:O3'	2.28	0.66
9:A:1105:U:N3	9:A:1108:A:OP2	2.29	0.66
30:a:529:A:OP2	41:m:126:SER:OG	2.08	0.66
37:i:12:THR:HG22	37:i:15:ARG:HH12	1.60	0.66
1:0:118:SER:OG	54:0:601:ATP:O3G	2.14	0.66
41:m:27:GLY:N	41:m:36:THR:O	2.29	0.66
9:A:1058:U:OP1	9:A:1074:U:O2'	2.14	0.65
32:d:21:LYS:O	39:k:94:SER:OG	2.11	0.65
9:A:987:C:O2	9:A:1023:G:O2'	2.13	0.65
17:N:120:GLU:OE1	22:S:65:SER:OG	2.06	0.65
25:V:40:ILE:O	25:V:44:THR:OG1	2.12	0.65
26:W:25:TYR:CE2	26:W:89:ILE:HB	2.31	0.65
1:0:348:GLY:CA	54:0:601:ATP:H5'2	2.27	0.65
14:J:42:ASP:O	14:J:45:SER:OG	2.12	0.65
30:a:1001:A:OP2	43:o:32:SER:OG	2.13	0.65
9:A:525:C:O2'	25:V:65:ASN:OD1	2.14	0.65
22:S:114:ARG:NH2	30:a:1468:A:O2'	2.30	0.65
30:a:227:A:O2'	30:a:228:A:O4'	2.06	0.65
30:a:165:G:O2'	30:a:1472:A:N3	2.26	0.65
9:A:2292:G:N7	28:Y:23:ARG:NH2	2.45	0.64
20:Q:8:ARG:O	20:Q:13:ARG:NH2	2.30	0.64
10:B:38:U:N3	10:B:42:G:OP2	2.30	0.64
11:G:13:ARG:NH1	11:G:16:MET:SD	2.70	0.64
34:f:77:VAL:O	34:f:80:THR:OG1	2.11	0.64
47:s:41:GLY:O	47:s:67:ARG:NH2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2123:G:O2'	9:A:2133:G:O4'	2.15	0.64
30:a:1020:G:O2'	30:a:1021:A:N7	2.31	0.64
47:s:23:GLU:OE2	47:s:58:LYS:NZ	2.30	0.64
9:A:1227:G:OP1	18:O:30:THR:OG1	2.16	0.63
9:A:1973:A:O2'	30:a:1511:U:O2'	2.10	0.63
30:a:1105:U:O2'	34:f:138:ARG:NH1	2.31	0.63
30:a:1178:G:OP1	39:k:70:HIS:ND1	2.31	0.63
13:I:63:LYS:NZ	13:I:67:GLN:OE1	2.31	0.63
53:3:16:ASP:O	53:3:20:GLY:N	2.31	0.63
9:A:1087:A:OP2	9:A:1149:G:N2	2.32	0.63
36:h:25:ARG:NH1	36:h:94:GLU:OE2	2.32	0.62
12:H:2:THR:OG1	12:H:85:ASN:O	2.09	0.62
20:Q:75:GLU:OE2	20:Q:78:GLU:N	2.32	0.62
1:0:445:ALA:HB3	1:0:448:TYR:HE1	1.64	0.62
9:A:602:U:OP1	18:O:29:LYS:NZ	2.32	0.62
9:A:2815:A:HO2'	9:A:2816:A:P	2.22	0.62
30:a:837:C:O2'	30:a:928:A:N1	2.31	0.62
31:c:20:THR:O	31:c:23:TRP:N	2.32	0.62
30:a:1120:A:O2'	30:a:1122:U:OP1	2.09	0.62
5:5:17:TYR:OH	9:A:2360:C:O2'	2.17	0.62
9:A:583:U:OP1	9:A:1255:G:O2'	2.10	0.61
9:A:1967:G:O2'	9:A:1969:U:O4	2.14	0.61
37:i:50:GLU:OE2	37:i:61:ARG:NH1	2.33	0.61
30:a:190:U:O2	30:a:230:G:O2'	2.12	0.61
30:a:845:A:O2'	30:a:846:U:OP1	2.17	0.61
30:a:977:U:O4	42:n:104:ASN:ND2	2.33	0.61
18:O:85:PHE:O	18:O:119:LYS:NZ	2.24	0.61
31:c:97:LEU:O	31:c:100:THR:OG1	2.13	0.61
9:A:1347:U:O4	26:W:59:ARG:NH1	2.34	0.61
9:A:2128:G:N1	9:A:2130:A:O2'	2.33	0.61
40:l:88:GLY:O	40:l:93:ARG:NH2	2.34	0.61
9:A:667:C:O2	9:A:677:U:O2'	2.19	0.61
30:a:527:C:OP1	41:m:127:ARG:NH2	2.31	0.61
9:A:1107:G:N3	9:A:1134:A:O2'	2.33	0.61
30:a:476:G:H5''	45:q:42:PRO:HB2	1.83	0.61
1:0:313:LEU:HD23	1:0:335:ILE:HD12	1.84	0.60
9:A:2790:G:OP2	9:A:2794:A:O2'	2.18	0.60
45:q:2:ALA:N	45:q:25:SER:HG	1.98	0.60
9:A:832:A:OP2	9:A:2084:A:O2'	2.19	0.60
13:I:78:ILE:HG23	13:I:79:ARG:HG2	1.83	0.60
30:a:1115:G:H21	30:a:1193:A:H62	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:382:A:N3	30:a:394:U:O2'	2.24	0.60
9:A:2291:A:OP2	28:Y:21:ASN:ND2	2.35	0.60
9:A:1591:G:OP2	9:A:1591:G:N2	2.30	0.60
9:A:2147:A:N3	9:A:2172:G:O2'	2.35	0.60
9:A:79:U:O2'	9:A:382:A:N3	2.31	0.60
9:A:1096:A:OP2	9:A:1128:G:N2	2.27	0.60
30:a:489:A:O2'	30:a:490:G:O5'	2.15	0.60
30:a:1127:C:N4	30:a:1130:C:OP1	2.35	0.60
9:A:1420:A:O2'	9:A:1431:U:O2	2.20	0.59
9:A:2815:A:O2'	9:A:2816:A:O5'	2.11	0.59
9:A:2764:G:OP2	15:K:2:SER:OG	2.19	0.59
10:B:25:A:N6	10:B:54:U:O4	2.34	0.59
52:F:52:PRO:O	52:F:58:GLN:NE2	2.36	0.59
9:A:1814:A:OP2	11:G:150:LYS:NZ	2.35	0.59
9:A:250:G:O2'	9:A:2445:A:OP1	2.11	0.59
9:A:288:U:O2'	9:A:289:U:O5'	2.18	0.59
9:A:1376:U:OP2	9:A:1429:U:O2'	2.15	0.59
11:G:107:PRO:HD2	11:G:110:LEU:HD22	1.84	0.59
9:A:1693:G:O2'	9:A:1694:C:O5'	2.20	0.59
9:A:1840:U:OP2	11:G:221:ARG:NH1	2.35	0.59
9:A:281:A:O2'	9:A:282:G:O5'	2.20	0.58
19:P:37:THR:OG1	19:P:128:LYS:O	2.16	0.58
30:a:693:G:OP1	30:a:758:C:O2'	2.18	0.58
9:A:1255:G:OP1	23:T:22:LYS:NZ	2.36	0.58
11:G:111:GLU:N	11:G:114:MET:SD	2.76	0.58
4:4:17:ARG:NE	9:A:1302:G:OP1	2.36	0.58
10:B:40:C:OP2	53:3:2:LYS:NZ	2.35	0.58
14:J:102:LYS:NZ	53:3:26:GLY:O	2.26	0.58
11:G:11:ASN:OD1	11:G:14:ARG:NH2	2.37	0.58
30:a:794:A:N3	30:a:1539:U:O2'	2.37	0.58
30:a:1000:G:O2'	43:o:29:ARG:NH2	2.36	0.58
10:B:54:U:O2'	10:B:56:A:N7	2.34	0.58
1:0:327:LEU:O	1:0:498:SER:OG	2.20	0.58
13:I:80:SER:HG	13:I:83:TRP:CD1	2.22	0.58
26:W:83:THR:OG1	26:W:86:SER:OG	2.14	0.58
30:a:453:C:O2'	30:a:567:G:OP1	2.21	0.58
37:i:29:ALA:HB2	37:i:60:ILE:HG22	1.86	0.58
45:q:18:TYR:O	45:q:39:THR:OG1	2.18	0.58
30:a:712:U:O4	30:a:729:G:O2'	2.21	0.58
9:A:2191:C:OP1	52:F:211:ASN:ND2	2.36	0.58
10:B:28:C:O3'	21:R:4:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:69:C:O2'	30:a:188:A:N3	2.34	0.58
9:A:1965:A:N3	9:A:2573:C:O2'	2.30	0.57
30:a:1486:C:OP1	49:u:26:ASN:ND2	2.37	0.57
33:e:126:ARG:NH1	33:e:128:ASP:OD2	2.37	0.57
38:j:9:THR:O	38:j:85:ARG:NH1	2.37	0.57
9:A:2670:A:O3'	15:K:160:LYS:NZ	2.37	0.57
11:G:204:ASN:OD1	11:G:205:ILE:N	2.37	0.57
30:a:429:C:OP2	33:e:67:GLN:NE2	2.37	0.57
7:7:16:ARG:NH2	7:7:62:LEU:O	2.36	0.57
34:f:163:GLU:O	37:i:116:LYS:NZ	2.36	0.57
9:A:1828:A:HO2'	9:A:1829:A:P	2.24	0.57
9:A:2181:G:N1	9:A:2184:A:OP2	2.36	0.57
9:A:2576:U:O2'	9:A:2578:A:N7	2.29	0.57
1:0:272:ARG:NH2	9:A:2449:G:O2'	2.37	0.57
9:A:1575:A:OP2	9:A:1583:G:N2	2.38	0.57
9:A:2262:U:N3	9:A:2266:G:OP2	2.35	0.57
9:A:2532:U:O4'	9:A:2555:A:N6	2.37	0.57
11:G:2:ALA:N	11:G:20:ASP:OD1	2.37	0.57
30:a:1239:A:O2'	30:a:1241:G:N7	2.35	0.57
9:A:116:G:OP2	9:A:118:A:O2'	2.22	0.57
9:A:883:A:O2'	9:A:884:U:O4'	2.22	0.57
30:a:720:A:N1	30:a:813:A:O2'	2.38	0.57
9:A:2418:G:O2'	9:A:2424:A:N6	2.37	0.56
41:m:81:PRO:O	41:m:112:ARG:NH2	2.39	0.56
16:M:19:VAL:HG13	16:M:143:ILE:CG1	2.35	0.56
30:a:1292:G:N2	30:a:1295:A:OP2	2.24	0.56
9:A:2369:C:O3'	28:Y:29:ARG:NH1	2.38	0.56
9:A:180:G:O2'	9:A:181:U:O4'	2.24	0.56
9:A:345:A:N3	9:A:365:G:O2'	2.38	0.56
16:M:32:VAL:CG2	16:M:143:ILE:HD12	2.34	0.56
8:8:7:VAL:O	9:A:1070:G:O2'	2.24	0.56
30:a:917:G:O2'	30:a:933:G:O6	2.20	0.56
15:K:117:ALA:HB2	15:K:123:PHE:CE2	2.41	0.56
10:B:31:G:N2	10:B:33:U:O4	2.39	0.56
9:A:412:U:OP2	29:Z:52:ARG:NH2	2.39	0.56
17:N:104:ARG:N	17:N:122:LEU:OXT	2.39	0.56
30:a:1164:A:N6	30:a:1166:U:O2'	2.39	0.56
30:a:1346:C:O2	48:t:36:ARG:NH2	2.39	0.56
30:a:1564:U:OP1	47:s:47:ARG:NE	2.39	0.55
3:2:30:LYS:O	3:2:33:SER:OG	2.08	0.55
9:A:2064:A:N6	9:A:2627:A:O2'	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:719:G:OP1	40:l:127:ARG:NH2	2.38	0.55
9:A:231:U:O2'	9:A:232:U:OP2	2.21	0.55
30:a:1376:A:O2'	36:h:33:ASP:OD1	2.16	0.55
9:A:1211:A:N3	9:A:1214:A:N6	2.53	0.55
9:A:2696:C:OP1	22:S:51:ARG:NH1	2.39	0.55
11:G:76:ALA:HB2	11:G:96:TYR:CD1	2.42	0.55
30:a:589:A:O2'	30:a:592:G:O3'	2.24	0.55
30:a:978:G:O6	42:n:104:ASN:ND2	2.40	0.55
41:m:53:MET:SD	41:m:103:LEU:HD22	2.47	0.55
9:A:84:A:OP2	27:X:4:LYS:NZ	2.26	0.55
9:A:2594:G:OP2	9:A:2594:G:N2	2.34	0.55
30:a:1343:C:O2	48:t:37:ARG:NH2	2.40	0.55
31:c:119:ALA:O	31:c:124:GLY:N	2.39	0.55
37:i:17:ALA:HB2	37:i:25:LEU:HD21	1.89	0.55
47:s:57:ARG:O	47:s:60:THR:OG1	2.22	0.55
1:0:313:LEU:HD13	1:0:372:LEU:HD23	1.88	0.55
30:a:940:A:OP2	41:m:101:LYS:NZ	2.23	0.55
20:Q:107:ILE:HG23	20:Q:121:VAL:HG13	1.89	0.54
30:a:771:U:OP1	30:a:878:C:O2'	2.24	0.54
30:a:465:U:O2'	33:e:116:ASN:OD1	2.19	0.54
7:7:7:HIS:NE2	9:A:253:A:OP1	2.41	0.54
9:A:550:G:OP1	9:A:1270:U:O2'	2.21	0.54
30:a:1108:G:OP2	34:f:32:ARG:NH2	2.41	0.54
31:c:46:THR:O	31:c:50:VAL:HG23	2.07	0.54
9:A:793:U:O2'	9:A:1308:A:N1	2.40	0.54
9:A:1531:A:O2'	11:G:98:ASP:OD1	2.23	0.54
9:A:1731:A:OP2	9:A:1740:A:N6	2.38	0.54
30:a:427:C:O2'	30:a:647:A:N3	2.34	0.54
37:i:42:ARG:NH1	37:i:43:GLU:OE2	2.41	0.54
45:q:53:GLU:OE2	45:q:82:LYS:NZ	2.23	0.54
11:G:177:ASN:O	11:G:178:SER:OG	2.18	0.54
14:J:52:LYS:NZ	14:J:56:GLU:OE2	2.36	0.54
30:a:733:U:OP1	40:l:87:LYS:NZ	2.37	0.54
9:A:655:A:OP2	13:I:106:ARG:NH1	2.37	0.54
23:T:91:ASN:OD1	23:T:92:ARG:N	2.40	0.54
30:a:1276:A:OP1	38:j:69:GLY:N	2.40	0.54
9:A:251:C:OP2	9:A:2407:C:O2'	2.25	0.54
20:Q:76:GLU:N	20:Q:76:GLU:OE1	2.40	0.54
52:F:51:ASP:OD2	52:F:54:LYS:NZ	2.24	0.54
9:A:754:A:N6	44:p:53:TYR:OH	2.36	0.54
9:A:1484:A:O2'	9:A:1485:A:N7	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2736:C:OP2	12:H:115:LYS:NZ	2.41	0.54
30:a:1314:A:N3	30:a:1378:C:O2'	2.37	0.54
9:A:1033:C:O2'	24:U:10:LYS:NZ	2.23	0.53
14:J:110:ARG:NH2	53:3:49:GLU:H	2.07	0.53
30:a:1265:A:O2'	36:h:114:HIS:O	2.19	0.53
9:A:1003:C:O2'	9:A:2286:A:N3	2.35	0.53
9:A:1109:A:O2'	9:A:1136:U:O5'	2.26	0.53
33:e:149:ILE:HG13	33:e:152:ILE:HG22	1.90	0.53
9:A:24:G:O2'	25:V:83:GLU:O	2.26	0.53
30:a:1371:U:OP1	38:j:122:ARG:NH2	2.42	0.53
34:f:77:VAL:N	34:f:80:THR:O	2.38	0.53
23:T:76:TYR:OH	23:T:92:ARG:NE	2.35	0.53
30:a:573:A:OP2	33:e:2:SER:N	2.42	0.53
30:a:860:U:OP1	47:s:46:ARG:NH2	2.39	0.53
30:a:712:U:O2'	30:a:729:G:N2	2.41	0.53
9:A:185:C:O2'	9:A:471:A:N3	2.37	0.53
30:a:119:U:OP1	49:u:12:ARG:NH1	2.38	0.53
1:0:39:ARG:O	1:0:44:LYS:NZ	2.42	0.53
9:A:1710:A:O2'	9:A:1716:G:N7	2.26	0.53
9:A:1978:C:OP1	9:A:1979:A:O2'	2.26	0.53
52:F:207:GLN:NE2	52:F:209:ILE:O	2.41	0.53
9:A:26:G:N1	9:A:551:A:OP2	2.42	0.53
12:H:195:ALA:O	12:H:198:SER:OG	2.21	0.53
32:d:69:THR:HG22	32:d:71:LYS:H	1.74	0.53
9:A:1302:G:OP2	25:V:20:ARG:NH2	2.42	0.52
45:q:72:ASN:O	45:q:75:SER:OG	2.22	0.52
30:a:703:U:H3	30:a:739:G:H22	1.57	0.52
2:1:44:LYS:NZ	9:A:75:G:OP1	2.42	0.52
9:A:3:U:O4	9:A:2911:C:O3'	2.22	0.52
18:O:11:GLY:O	18:O:14:GLN:NE2	2.43	0.52
9:A:2756:C:OP2	9:A:2768:C:N4	2.43	0.52
9:A:2808:U:N3	9:A:2809:U:O2	2.42	0.52
30:a:526:G:O3'	41:m:134:ARG:NH2	2.42	0.52
30:a:1303:C:O2'	30:a:1305:A:N3	2.31	0.52
12:H:13:THR:HG22	22:S:5:ILE:HG23	1.92	0.52
9:A:1767:C:N3	9:A:2729:U:O2'	2.36	0.52
1:0:100:LEU:O	1:0:103:LEU:C	2.53	0.52
14:J:126:GLY:O	14:J:158:THR:OG1	2.28	0.52
30:a:994:C:OP2	30:a:995:A:O2'	2.09	0.52
30:a:1088:G:N7	32:d:3:GLN:NE2	2.58	0.52
4:4:16:ARG:NH2	9:A:1300:G:OP1	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1813:C:OP1	11:G:182:ARG:NH2	2.43	0.51
21:R:8:ASN:OD1	21:R:11:ARG:NH2	2.43	0.51
9:A:565:C:N4	9:A:2792:U:OP2	2.37	0.51
1:O:382:ARG:N	1:O:436:GLU:OE2	2.38	0.51
9:A:782:A:O2'	9:A:1701:U:OP1	2.25	0.51
10:B:41:C:O2	14:J:92:ARG:NH1	2.43	0.51
44:p:18:HIS:ND1	44:p:21:ASP:OD2	2.40	0.51
52:F:216:THR:OG1	52:F:219:GLY:N	2.43	0.51
9:A:1642:C:OP1	26:W:76:ARG:NH2	2.40	0.51
9:A:1939:U:O2'	9:A:1941:A:N7	2.40	0.51
13:I:40:GLN:NE2	13:I:182:SER:OG	2.38	0.51
24:U:32:LYS:NZ	24:U:98:GLU:OE1	2.44	0.51
30:a:1386:A:OP2	43:o:35:ARG:NH2	2.43	0.51
9:A:2535:U:O2'	9:A:2660:U:OP1	2.25	0.51
10:B:35:C:O2	21:R:101:HIS:NE2	2.43	0.51
30:a:994:C:H4'	38:j:127:PHE:HE1	1.75	0.51
27:X:72:ASP:OD1	27:X:94:SER:OG	2.27	0.51
30:a:475:A:H3'	30:a:476:G:H8	1.75	0.51
30:a:1203:G:O5'	38:j:99:LYS:NZ	2.44	0.51
9:A:995:G:O6	9:A:997:U:O2'	2.27	0.51
37:i:24:THR:OG1	37:i:62:VAL:O	2.18	0.51
52:F:51:ASP:N	52:F:57:GLN:OE1	2.39	0.51
1:O:219:ILE:HG21	1:O:287:LYS:HB2	1.92	0.51
9:A:2011:A:OP2	12:H:141:ARG:NH1	2.41	0.50
30:a:1100:U:O2	31:c:103:ASN:ND2	2.44	0.50
9:A:1390:G:OP2	11:G:38:LYS:NZ	2.40	0.50
11:G:208:ALA:O	11:G:211:SER:OG	2.27	0.50
26:W:34:ASN:OD1	26:W:35:LYS:N	2.44	0.50
30:a:1328:U:OP2	42:n:21:TYR:OH	2.15	0.50
2:1:49:SER:OG	2:1:52:ARG:NH2	2.45	0.50
9:A:1691:G:O2'	20:Q:116:ASP:OD2	2.30	0.50
13:I:150:THR:HG22	13:I:151:LYS:H	1.75	0.50
7:7:57:ARG:NH2	18:O:51:GLU:OE2	2.44	0.50
9:A:1050:A:OP2	23:T:66:ASN:ND2	2.45	0.50
9:A:1644:U:OP1	26:W:59:ARG:NH2	2.45	0.50
9:A:1831:U:OP2	11:G:87:ARG:NH1	2.43	0.50
30:a:806:A:N6	30:a:827:U:OP2	2.42	0.50
30:a:1088:G:OP1	39:k:53:ARG:NH2	2.43	0.50
50:D:22:A:O2'	50:D:23:G:O5'	2.30	0.50
9:A:600:C:O3'	24:U:76:TYR:OH	2.30	0.50
30:a:980:G:H5''	30:a:992:A:H61	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:69:MET:HE3	27:X:78:ALA:HB3	1.92	0.50
30:a:174:U:O2'	30:a:175:G:O5'	2.24	0.50
34:f:83:HIS:CD2	37:i:98:LEU:HD22	2.47	0.50
30:a:24:G:O2'	30:a:940:A:N1	2.38	0.50
9:A:1095:G:N1	9:A:1141:C:OP2	2.45	0.50
9:A:2236:A:OP1	11:G:171:TYR:OH	2.24	0.50
10:B:32:U:O2'	10:B:42:G:N7	2.32	0.50
30:a:973:A:O2'	30:a:1359:A:O2'	2.23	0.50
30:a:1153:U:OP1	39:k:7:ARG:NH1	2.45	0.50
30:a:701:A:H61	30:a:741:A:H61	1.60	0.49
30:a:815:U:O2'	30:a:817:G:N7	2.42	0.49
7:7:52:LYS:NZ	9:A:976:C:OP2	2.39	0.49
30:a:685:C:OP1	44:p:5:GLN:NE2	2.44	0.49
9:A:59:G:OP1	26:W:73:LYS:NZ	2.28	0.49
39:k:51:VAL:HG13	43:o:41:ARG:HB2	1.93	0.49
17:N:97:ARG:NH2	30:a:365:C:OP2	2.40	0.49
33:e:46:GLU:OE1	34:f:112:ARG:NH2	2.46	0.49
4:4:39:SER:HG	9:A:2825:C:HO2'	1.58	0.49
9:A:846:U:OP2	18:O:41:ARG:NH2	2.45	0.49
26:W:25:TYR:HE2	26:W:89:ILE:HB	1.74	0.49
30:a:938:U:OP2	41:m:107:ARG:NH2	2.40	0.49
9:A:2883:A:O2'	9:A:2884:C:OP1	2.26	0.49
27:X:9:VAL:HG13	27:X:68:VAL:HG13	1.95	0.49
30:a:75:U:N3	30:a:112:A:N7	2.61	0.49
1:0:348:GLY:C	54:0:601:ATP:H5'2	2.37	0.49
30:a:973:A:HO2'	30:a:1359:A:HO2'	1.56	0.49
42:n:17:VAL:C	42:n:20:THR:HG1	2.20	0.49
52:F:34:ASN:OD1	52:F:35:ILE:N	2.46	0.49
53:3:16:ASP:OD2	53:3:51:THR:HG22	2.13	0.49
9:A:2858:G:O2'	9:A:2859:G:O5'	2.27	0.48
22:S:14:ARG:NH1	22:S:78:THR:O	2.46	0.48
30:a:971:G:N1	30:a:1364:G:OP2	2.42	0.48
37:i:115:ASP:OD1	37:i:116:LYS:N	2.46	0.48
9:A:641:G:O6	18:O:103:LYS:NZ	2.39	0.48
9:A:1984:A:O2'	9:A:1985:G:OP1	2.31	0.48
40:l:21:ALA:N	40:l:83:ASP:O	2.42	0.48
7:7:13:ARG:NH1	18:O:58:PHE:O	2.42	0.48
9:A:1494:A:O2'	9:A:2715:G:O6	2.26	0.48
9:A:2304:U:O2'	9:A:2387:C:O2	2.31	0.48
25:V:30:ARG:NH2	25:V:79:ALA:O	2.47	0.48
32:d:179:ALA:HB1	32:d:181:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:244:LYS:NZ	9:A:2264:G:O6	2.35	0.48
9:A:2598:U:O2	9:A:2598:U:O4'	2.29	0.48
14:J:25:VAL:O	14:J:28:THR:OG1	2.13	0.48
15:K:52:PHE:O	15:K:65:HIS:NE2	2.44	0.48
1:0:383:GLN:NE2	54:0:601:ATP:O2G	2.33	0.48
30:a:1337:A:OP1	53:3:73:ARG:NH2	2.41	0.48
48:t:49:ILE:HD11	48:t:71:LEU:HD22	1.93	0.48
9:A:575:A:OP1	9:A:1034:C:N4	2.46	0.48
9:A:1192:C:OP1	23:T:92:ARG:NH2	2.47	0.48
9:A:2859:G:O6	22:S:21:ARG:NH2	2.44	0.48
9:A:281:A:HO2'	9:A:282:G:P	2.37	0.48
47:s:37:ILE:HG22	47:s:38:SER:O	2.13	0.48
20:Q:75:GLU:OE1	20:Q:80:ILE:N	2.47	0.48
9:A:75:G:O2'	9:A:76:C:OP2	2.26	0.47
9:A:2316:G:O2'	14:J:129:THR:OG1	2.23	0.47
9:A:2859:G:OP1	22:S:93:ARG:NE	2.34	0.47
10:B:3:U:OP1	10:B:59:U:O2'	2.22	0.47
14:J:136:LEU:HA	14:J:141:VAL:HG11	1.95	0.47
10:B:49:G:O2'	10:B:50:A:O5'	2.23	0.47
9:A:515:G:N1	9:A:518:A:OP2	2.44	0.47
16:M:32:VAL:O	16:M:35:SER:OG	2.25	0.47
30:a:553:G:O2'	30:a:561:A:N1	2.41	0.47
43:o:26:ARG:NH1	43:o:43:CYS:SG	2.82	0.47
2:1:48:GLN:NE2	9:A:76:C:OP1	2.47	0.47
9:A:613:G:O2'	9:A:1290:A:OP1	2.33	0.47
9:A:2349:A:H61	28:Y:52:THR:CG2	2.27	0.47
5:5:19:THR:OG1	9:A:2299:A:N6	2.48	0.47
9:A:739:G:O2'	9:A:1674:A:N3	2.44	0.47
9:A:1318:G:N2	9:A:1321:A:OP2	2.47	0.47
30:a:907:C:OP1	41:m:5:ASN:ND2	2.47	0.47
30:a:1340:C:C6	48:t:5:LEU:HD21	2.49	0.47
33:e:121:THR:N	33:e:141:GLY:O	2.47	0.47
44:p:33:THR:HG22	44:p:63:ARG:HH11	1.80	0.47
47:s:46:ARG:NH1	47:s:53:ALA:HB2	2.30	0.47
30:a:1108:G:OP2	34:f:52:LYS:NZ	2.41	0.47
9:A:1357:A:N1	9:A:1368:C:O2'	2.38	0.47
40:l:83:ASP:OD1	40:l:84:VAL:N	2.48	0.47
1:0:92:GLU:HB2	1:0:95:LYS:HB2	1.96	0.46
9:A:1321:A:O2'	9:A:1323:U:OP2	2.31	0.46
31:c:33:THR:O	31:c:40:ILE:N	2.42	0.46
30:a:1254:C:O2'	42:n:115:THR:O	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1444:A:N6	30:a:1509:G:O2'	2.46	0.46
33:e:127:VAL:HG12	33:e:129:ILE:H	1.80	0.46
8:8:29:ALA:O	15:K:170:ARG:NH1	2.48	0.46
9:A:680:G:N2	9:A:683:U:OP2	2.38	0.46
9:A:2138:G:O2'	9:A:2186:A:N6	2.46	0.46
22:S:114:ARG:NH2	30:a:1469:G:O4'	2.42	0.46
30:a:1079:U:O2'	30:a:1082:A:OP2	2.15	0.46
30:a:1227:A:O2'	30:a:1228:U:OP2	2.33	0.46
46:r:51:ASP:OD2	46:r:55:THR:N	2.48	0.46
9:A:2284:G:OP1	28:Y:27:SER:OG	2.23	0.46
30:a:903:A:H1'	37:i:12:THR:HG21	1.96	0.46
3:2:18:ASN:OD1	3:2:19:GLN:N	2.47	0.46
30:a:285:G:OP1	49:u:77:ARG:NE	2.42	0.46
9:A:27:G:O2'	9:A:28:A:O5'	2.26	0.46
9:A:769:A:OP1	9:A:1788:U:O2'	2.28	0.46
47:s:51:THR:OG1	47:s:56:GLN:OE1	2.33	0.46
30:a:1275:C:O2'	38:j:75:GLN:NE2	2.49	0.46
48:t:6:LYS:NZ	53:3:77:LYS:O	2.48	0.46
37:i:40:LEU:HB2	37:i:46:ILE:HD12	1.97	0.46
39:k:52:ILE:HG22	39:k:54:ALA:H	1.80	0.46
9:A:492:A:N3	9:A:496:A:O2'	2.49	0.46
9:A:922:G:N1	9:A:935:U:O4	2.49	0.46
30:a:1101:G:O2'	31:c:102:THR:OG1	2.30	0.46
9:A:895:G:O2'	28:Y:36:ASP:OD2	2.29	0.46
30:a:139:C:OP1	30:a:337:C:O2'	2.33	0.46
11:G:76:ALA:HB2	11:G:96:TYR:CE1	2.52	0.45
13:I:101:PHE:O	13:I:106:ARG:NE	2.47	0.45
30:a:966:G:O5'	36:h:102:ARG:NH1	2.49	0.45
33:e:169:ASP:OD1	33:e:170:THR:N	2.48	0.45
9:A:857:G:N1	9:A:1225:U:OP2	2.45	0.45
9:A:2188:U:O2'	52:F:219:GLY:O	2.33	0.45
10:B:11:A:N6	10:B:67:G:O2'	2.50	0.45
33:e:93:GLN:OE1	33:e:133:HIS:NE2	2.50	0.45
40:l:81:THR:HG22	40:l:106:GLU:HB3	1.97	0.45
48:t:42:PRO:HG3	53:3:71:VAL:HG13	1.98	0.45
1:0:298:ASP:OD1	1:0:299:SER:N	2.48	0.45
5:5:1:MET:SD	5:5:22:ASN:ND2	2.84	0.45
9:A:572:U:O2'	23:T:49:ASP:OD2	2.27	0.45
37:i:29:ALA:HB2	37:i:60:ILE:CG2	2.46	0.45
37:i:55:ASP:OD1	37:i:56:LYS:N	2.49	0.45
9:A:1936:U:OP1	50:D:25:U:O2'	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:n:66:GLU:OE2	42:n:70:ARG:NH2	2.49	0.45
9:A:225:A:N1	9:A:446:C:O2'	2.47	0.45
30:a:1099:G:OP1	34:f:62:LYS:NZ	2.47	0.45
32:d:11:ARG:NH2	32:d:174:LEU:O	2.46	0.45
14:J:98:GLU:OE1	53:3:9:TYR:OH	2.29	0.45
9:A:829:A:H62	13:I:66:ARG:CZ	2.30	0.45
9:A:1804:A:N6	9:A:1841:G:O2'	2.50	0.45
9:A:2128:G:O2'	9:A:2184:A:N6	2.50	0.45
9:A:2801:C:O2'	9:A:2819:A:N3	2.35	0.45
14:J:34:ILE:HD11	14:J:100:LEU:HD12	1.99	0.45
30:a:690:G:H22	30:a:767:G:H1	1.64	0.45
30:a:1004:A:O2'	30:a:1249:C:N4	2.50	0.45
41:m:70:LEU:HD11	41:m:76:VAL:HG21	1.99	0.45
1:0:101:THR:OG1	9:A:2125:A:N3	2.49	0.45
9:A:519:A:O4'	27:X:41:VAL:HG21	2.15	0.45
30:a:601:G:O2'	30:a:847:G:OP2	2.28	0.45
2:1:21:LEU:HD12	2:1:46:VAL:HG13	1.99	0.45
9:A:2008:U:O2	17:N:3:GLN:NE2	2.42	0.45
9:A:2349:A:H61	28:Y:52:THR:HG21	1.81	0.45
12:H:6:LEU:HD12	12:H:199:LEU:HD11	1.98	0.44
30:a:981:G:H21	30:a:1253:A:H62	1.64	0.44
3:2:18:ASN:O	3:2:22:THR:HG23	2.17	0.44
3:2:22:THR:HG22	9:A:890:A:O2'	2.18	0.44
33:e:53:GLU:HG3	33:e:194:LEU:HD12	1.98	0.44
9:A:901:A:N3	10:B:77:G:O2'	2.48	0.44
9:A:1125:A:O2'	9:A:1126:G:N7	2.43	0.44
40:l:67:ALA:O	40:l:71:THR:HG23	2.17	0.44
9:A:1792:U:OP2	9:A:1797:A:N6	2.48	0.44
12:H:54:GLN:O	12:H:78:ARG:N	2.44	0.44
21:R:95:ARG:NH1	21:R:98:TYR:O	2.47	0.44
9:A:1132:G:N2	9:A:1138:G:O6	2.51	0.44
9:A:1455:G:H2'	9:A:1627:G:H22	1.82	0.44
9:A:2849:G:N2	20:Q:101:GLN:O	2.45	0.44
13:I:156:LEU:O	13:I:178:SER:OG	2.27	0.44
9:A:2046:A:O2'	9:A:2048:G:OP2	2.31	0.44
21:R:30:ARG:HH21	21:R:45:ILE:HG21	1.82	0.44
30:a:350:G:N1	30:a:353:A:OP2	2.51	0.44
30:a:1105:U:O3'	34:f:138:ARG:NH1	2.38	0.44
9:A:1065:A:OP2	9:A:1173:C:O2'	2.23	0.44
9:A:2902:G:H1'	9:A:2903:G:H21	1.83	0.43
13:I:133:ALA:HB1	13:I:134:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1000:G:OP1	39:k:59:LYS:NZ	2.47	0.43
9:A:1850:C:O2'	9:A:1940:A:N3	2.47	0.43
9:A:1932:A:N1	30:a:1522:U:O2'	2.46	0.43
40:l:29:ASN:OD1	40:l:30:THR:N	2.52	0.43
9:A:2026:A:O2'	25:V:99:SER:OG	2.01	0.43
25:V:74:LEU:HD23	25:V:112:VAL:HG22	2.00	0.43
30:a:713:A:N1	30:a:726:G:O2'	2.50	0.43
1:0:85:LEU:HD22	1:0:129:LEU:HD21	1.99	0.43
4:4:53:ASP:OD1	4:4:54:VAL:N	2.52	0.43
9:A:1302:G:O2'	9:A:2025:G:O6	2.34	0.43
11:G:142:HIS:N	11:G:191:THR:O	2.41	0.43
13:I:155:VAL:HG12	13:I:198:ALA:HB1	2.00	0.43
31:c:34:GLU:N	31:c:34:GLU:OE1	2.51	0.43
33:e:115:VAL:HG11	33:e:130:PRO:HA	2.00	0.43
2:1:29:ARG:NH2	26:W:4:LEU:O	2.51	0.43
20:Q:75:GLU:OE2	20:Q:77:ASP:N	2.51	0.43
23:T:37:GLU:O	23:T:41:ASN:ND2	2.52	0.43
7:7:31:HIS:NE2	9:A:2405:A:OP1	2.51	0.43
9:A:1693:G:O2'	9:A:1694:C:O4'	2.37	0.43
11:G:97:GLU:OE2	11:G:115:ARG:NH1	2.52	0.43
33:e:23:GLY:O	33:e:27:ALA:N	2.51	0.43
9:A:1256:A:OP2	23:T:19:LYS:NZ	2.46	0.43
9:A:1575:A:OP2	9:A:1582:A:N6	2.52	0.43
9:A:2698:G:OP1	17:N:78:LYS:NZ	2.34	0.43
9:A:2808:U:O2'	9:A:2809:U:OP1	2.33	0.43
15:K:44:ASN:OD1	15:K:53:ILE:HD12	2.18	0.43
30:a:1033:C:HO2'	30:a:1034:A:P	2.40	0.43
42:n:81:MET:O	42:n:92:ARG:NH2	2.52	0.43
30:a:1402:U:O4	36:h:10:ARG:NH1	2.49	0.43
43:o:59:ALA:HB1	43:o:61:TRP:HZ3	1.84	0.43
47:s:34:LYS:HA	47:s:37:ILE:HD12	2.00	0.43
20:Q:17:LEU:O	20:Q:21:THR:HG23	2.19	0.43
31:c:54:TYR:CD1	31:c:220:ALA:HB2	2.54	0.43
1:0:6:LEU:HD12	1:0:26:ILE:HD11	1.99	0.43
9:A:604:U:O4	24:U:80:LYS:NZ	2.50	0.43
9:A:934:U:N3	9:A:935:U:O4	2.52	0.43
9:A:1224:G:OP1	24:U:84:ARG:NE	2.51	0.43
17:N:3:GLN:O	17:N:6:SER:OG	2.28	0.43
32:d:205:GLU:N	32:d:205:GLU:OE1	2.52	0.43
30:a:1113:U:H3	30:a:1126:G:H22	1.65	0.42
38:j:68:ASN:OD1	38:j:69:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:m:48:THR:N	41:m:67:ARG:O	2.49	0.42
19:P:119:ARG:O	19:P:122:SER:OG	2.30	0.42
28:Y:24:ASP:OD1	28:Y:25:SER:N	2.50	0.42
50:D:22:A:O2'	50:D:23:G:O4'	2.37	0.42
9:A:2875:U:OP2	9:A:2876:G:O2'	2.22	0.42
10:B:40:C:N3	14:J:90:THR:OG1	2.41	0.42
12:H:105:GLY:N	12:H:176:VAL:O	2.51	0.42
9:A:743:G:O2'	9:A:765:G:N2	2.50	0.42
22:S:14:ARG:NH1	22:S:81:VAL:O	2.50	0.42
22:S:39:ARG:NH2	30:a:371:C:OP1	2.46	0.42
30:a:1519:A:OP1	41:m:57:LYS:N	2.52	0.42
37:i:8:ALA:O	37:i:12:THR:HG23	2.19	0.42
30:a:1042:G:O2'	30:a:1244:C:O2'	2.33	0.42
37:i:47:ARG:NH1	37:i:64:LEU:O	2.50	0.42
1:0:121:GLU:O	1:0:125:VAL:HG23	2.19	0.42
9:A:538:G:N1	9:A:541:A:OP2	2.46	0.42
9:A:585:A:O2'	9:A:586:U:O5'	2.38	0.42
9:A:1948:G:N2	9:A:1975:C:O2'	2.50	0.42
44:p:22:THR:O	44:p:27:VAL:HG11	2.19	0.42
1:0:181:ASP:O	1:0:196:GLY:N	2.51	0.42
5:5:22:ASN:ND2	9:A:2298:C:OP2	2.48	0.42
9:A:2012:C:OP1	9:A:2736:C:O2'	2.34	0.42
9:A:2525:C:O2	12:H:145:SER:OG	2.37	0.42
14:J:34:ILE:HD12	14:J:96:MET:HG2	2.01	0.42
14:J:49:ASN:OD1	14:J:50:LEU:N	2.52	0.42
30:a:399:A:O2'	30:a:477:A:N7	2.52	0.42
34:f:25:VAL:HG12	34:f:26:LYS:N	2.34	0.42
1:0:216:ASN:ND2	1:0:291:LEU:HD11	2.34	0.42
9:A:83:G:N2	9:A:102:A:OP2	2.26	0.42
9:A:1913:A:O2'	9:A:1914:A:OP1	2.35	0.42
14:J:52:LYS:NZ	14:J:145:LEU:O	2.50	0.42
20:Q:107:ILE:HG23	20:Q:121:VAL:CG1	2.49	0.42
6:6:33:SER:OG	9:A:506:G:OP1	2.20	0.42
9:A:99:A:OP1	9:A:100:U:O2'	2.26	0.42
9:A:197:A:H61	9:A:200:C:H3'	1.85	0.42
16:M:19:VAL:HG13	16:M:143:ILE:HG13	2.02	0.42
40:l:113:VAL:HG12	40:l:113:VAL:O	2.20	0.42
31:c:86:ARG:NH1	31:c:219:ASP:OD1	2.52	0.42
9:A:2138:G:H22	9:A:2185:U:C5'	2.33	0.41
12:H:9:LYS:HB2	12:H:200:ILE:HD11	2.01	0.41
30:a:1146:U:OP1	38:j:85:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:n:23:TYR:CE2	42:n:69:LEU:HD22	2.55	0.41
28:Y:81:LYS:N	28:Y:85:LYS:O	2.45	0.41
30:a:1122:U:P	30:a:1135:G:H22	2.44	0.41
35:g:81:ASP:OD1	35:g:93:HIS:NE2	2.45	0.41
9:A:2649:U:HO2'	12:H:46:TYR:HH	1.59	0.41
14:J:17:VAL:HG23	14:J:22:TYR:HB2	2.03	0.41
31:c:164:VAL:HG23	31:c:165:ASP:N	2.35	0.41
37:i:29:ALA:HB3	37:i:58:GLY:O	2.20	0.41
40:l:36:ASP:OD1	40:l:37:THR:N	2.52	0.41
9:A:203:C:OP1	29:Z:18:ARG:NH2	2.54	0.41
14:J:37:ASN:OD1	14:J:38:MET:N	2.53	0.41
16:M:19:VAL:HG13	16:M:143:ILE:HG12	2.02	0.41
25:V:51:ILE:HD12	25:V:51:ILE:H	1.85	0.41
30:a:662:U:OP1	46:r:9:LYS:NZ	2.51	0.41
30:a:783:U:O2'	30:a:906:C:O2	2.36	0.41
9:A:1331:A:OP1	9:A:2722:G:O2'	2.34	0.41
15:K:20:ASP:OD1	15:K:21:GLY:N	2.48	0.41
20:Q:73:VAL:HG13	20:Q:73:VAL:O	2.20	0.41
30:a:522:G:H21	30:a:523:A:H3'	1.85	0.41
1:0:327:LEU:HD21	54:0:601:ATP:H5'1	2.03	0.41
9:A:668:G:N2	9:A:671:A:OP2	2.45	0.41
21:R:68:LYS:O	21:R:71:THR:OG1	2.33	0.41
39:k:50:THR:HG22	39:k:64:GLN:HG2	2.01	0.41
6:6:8:ASN:ND2	9:A:809:G:OP1	2.46	0.41
9:A:2452:A:O2'	9:A:2613:A:OP1	2.18	0.41
25:V:9:LYS:HG2	25:V:111:VAL:HG22	2.02	0.41
30:a:320:C:OP1	30:a:636:G:O2'	2.26	0.41
7:7:41:ARG:NH1	9:A:2432:U:OP1	2.48	0.41
10:B:70:G:O2'	10:B:71:A:O4'	2.36	0.41
11:G:16:MET:HE1	11:G:207:LYS:HE2	2.02	0.41
13:I:187:VAL:HG13	18:O:1:MET:O	2.21	0.41
30:a:1217:A:OP2	32:d:2:GLY:N	2.54	0.41
37:i:108:THR:HG22	37:i:124:GLY:O	2.21	0.41
39:k:97:ASN:OD1	39:k:98:ILE:N	2.54	0.41
1:0:307:THR:OG1	1:0:446:GLU:OE2	2.34	0.41
7:7:8:ARG:NH2	9:A:246:A:OP2	2.44	0.41
9:A:3:U:O4	9:A:2911:C:O2'	2.26	0.41
9:A:50:U:HO2'	9:A:51:G:P	2.43	0.41
9:A:641:G:N3	9:A:696:U:O2'	2.54	0.41
9:A:1358:G:OP1	25:V:103:LYS:NZ	2.31	0.41
9:A:2463:A:OP1	9:A:2510:A:O2'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1266:U:OP1	36:h:119:ARG:NH2	2.54	0.41
30:a:1341:U:O2'	30:a:1386:A:N3	2.37	0.41
34:f:83:HIS:HD2	37:i:98:LEU:HD22	1.85	0.41
37:i:12:THR:HG22	37:i:15:ARG:NH1	2.32	0.41
37:i:76:ASN:OD1	37:i:77:LEU:N	2.53	0.41
40:l:50:LEU:HD21	40:l:66:ALA:HA	2.03	0.41
49:u:21:ASN:HD22	49:u:65:LEU:HD21	1.86	0.41
3:2:28:LEU:HD21	3:2:35:VAL:HG12	2.02	0.41
12:H:17:THR:OG1	12:H:23:ILE:HD12	2.20	0.41
30:a:791:G:N1	30:a:838:G:O2'	2.46	0.41
32:d:113:LYS:NZ	32:d:117:GLU:OE2	2.53	0.40
9:A:823:U:O2'	9:A:824:U:OP2	2.35	0.40
15:K:54:ARG:NH2	15:K:57:ASP:OD1	2.52	0.40
30:a:903:A:C1'	37:i:12:THR:HG21	2.51	0.40
31:c:20:THR:O	31:c:22:ARG:N	2.54	0.40
32:d:8:ILE:O	32:d:12:VAL:HG23	2.22	0.40
37:i:92:ASP:OD1	37:i:93:GLU:N	2.54	0.40
9:A:566:A:OP2	16:M:114:THR:HG23	2.21	0.40
17:N:63:VAL:CG2	17:N:102:VAL:HG22	2.50	0.40
21:R:59:LEU:O	21:R:59:LEU:HD23	2.21	0.40
30:a:1248:G:OP2	30:a:1348:C:N4	2.45	0.40
31:c:131:LYS:HA	31:c:134:VAL:HG12	2.03	0.40
9:A:714:A:N3	9:A:2456:U:O2'	2.45	0.40
9:A:1405:C:O3'	11:G:45:ASN:ND2	2.45	0.40
11:G:124:ILE:HG23	11:G:124:ILE:O	2.22	0.40
30:a:704:U:O2'	30:a:804:G:OP1	2.35	0.40
30:a:818:A:O2'	30:a:820:A:N7	2.50	0.40
30:a:1104:G:N1	30:a:1107:A:OP2	2.48	0.40
33:e:99:VAL:HB	33:e:111:ALA:HB1	2.03	0.40
35:g:25:LEU:HD21	35:g:90:ILE:HD11	2.03	0.40
10:B:27:A:OP2	21:R:36:SER:OG	2.20	0.40
30:a:176:G:N2	30:a:179:A:OP2	2.49	0.40
33:e:98:VAL:HG11	33:e:140:ILE:HG13	2.04	0.40
35:g:50:ARG:NE	35:g:60:GLU:OE2	2.55	0.40
46:r:16:VAL:HG21	46:r:27:VAL:HG21	2.02	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	493/541 (91%)	468 (95%)	25 (5%)	0	100	100
2	1	57/62 (92%)	57 (100%)	0	0	100	100
3	2	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
4	4	51/59 (86%)	46 (90%)	5 (10%)	0	100	100
5	5	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
6	6	41/44 (93%)	41 (100%)	0	0	100	100
7	7	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
8	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	G	272/276 (99%)	252 (93%)	20 (7%)	0	100	100
12	H	205/209 (98%)	193 (94%)	12 (6%)	0	100	100
13	I	203/207 (98%)	188 (93%)	15 (7%)	0	100	100
14	J	174/179 (97%)	163 (94%)	11 (6%)	0	100	100
15	K	172/178 (97%)	160 (93%)	12 (7%)	0	100	100
16	M	143/147 (97%)	134 (94%)	9 (6%)	0	100	100
17	N	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
18	O	144/146 (99%)	130 (90%)	14 (10%)	0	100	100
19	P	132/144 (92%)	128 (97%)	4 (3%)	0	100	100
20	Q	123/127 (97%)	114 (93%)	9 (7%)	0	100	100
21	R	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
22	S	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
23	T	114/119 (96%)	110 (96%)	4 (4%)	0	100	100
24	U	99/102 (97%)	94 (95%)	5 (5%)	0	100	100
25	V	109/115 (95%)	104 (95%)	5 (5%)	0	100	100
26	W	89/96 (93%)	87 (98%)	2 (2%)	0	100	100
27	X	99/103 (96%)	91 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Y	72/95 (76%)	68 (94%)	4 (6%)	0	100	100
29	Z	58/62 (94%)	52 (90%)	6 (10%)	0	100	100
31	c	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
32	d	204/218 (94%)	189 (93%)	15 (7%)	0	100	100
33	e	198/203 (98%)	187 (94%)	11 (6%)	0	100	100
34	f	161/166 (97%)	149 (92%)	12 (8%)	0	100	100
35	g	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
36	h	151/156 (97%)	145 (96%)	6 (4%)	0	100	100
37	i	129/132 (98%)	116 (90%)	13 (10%)	0	100	100
38	j	126/130 (97%)	114 (90%)	12 (10%)	0	100	100
39	k	94/102 (92%)	90 (96%)	4 (4%)	0	100	100
40	l	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
41	m	133/137 (97%)	117 (88%)	16 (12%)	0	100	100
42	n	112/121 (93%)	102 (91%)	10 (9%)	0	100	100
43	o	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
44	p	83/89 (93%)	81 (98%)	2 (2%)	0	100	100
45	q	85/91 (93%)	79 (93%)	6 (7%)	0	100	100
46	r	79/88 (90%)	68 (86%)	11 (14%)	0	100	100
47	s	64/79 (81%)	60 (94%)	4 (6%)	0	100	100
48	t	79/92 (86%)	72 (91%)	7 (9%)	0	100	100
49	u	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
52	F	126/229 (55%)	119 (94%)	7 (6%)	0	100	100
53	3	49/89 (55%)	48 (98%)	1 (2%)	0	100	100
All	All	5834/6334 (92%)	5463 (94%)	371 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	435/473 (92%)	435 (100%)	0	100	100
2	1	54/56 (96%)	54 (100%)	0	100	100
3	2	48/50 (96%)	48 (100%)	0	100	100
4	4	43/48 (90%)	43 (100%)	0	100	100
5	5	48/49 (98%)	48 (100%)	0	100	100
6	6	39/39 (100%)	39 (100%)	0	100	100
7	7	51/53 (96%)	51 (100%)	0	100	100
8	8	35/35 (100%)	35 (100%)	0	100	100
11	G	224/226 (99%)	223 (100%)	1 (0%)	84	94
12	H	170/172 (99%)	170 (100%)	0	100	100
13	I	172/173 (99%)	172 (100%)	0	100	100
14	J	153/156 (98%)	153 (100%)	0	100	100
15	K	145/148 (98%)	145 (100%)	0	100	100
16	M	122/124 (98%)	122 (100%)	0	100	100
17	N	98/98 (100%)	98 (100%)	0	100	100
18	O	112/112 (100%)	112 (100%)	0	100	100
19	P	107/114 (94%)	107 (100%)	0	100	100
20	Q	107/109 (98%)	107 (100%)	0	100	100
21	R	91/92 (99%)	91 (100%)	0	100	100
22	S	97/98 (99%)	97 (100%)	0	100	100
23	T	92/95 (97%)	92 (100%)	0	100	100
24	U	83/83 (100%)	83 (100%)	0	100	100
25	V	94/98 (96%)	94 (100%)	0	100	100
26	W	82/85 (96%)	82 (100%)	0	100	100
27	X	85/87 (98%)	85 (100%)	0	100	100
28	Y	59/75 (79%)	59 (100%)	0	100	100
29	Z	53/55 (96%)	53 (100%)	0	100	100
31	c	187/220 (85%)	187 (100%)	0	100	100
32	d	164/174 (94%)	164 (100%)	0	100	100
33	e	174/177 (98%)	174 (100%)	0	100	100
34	f	125/128 (98%)	125 (100%)	0	100	100
35	g	86/88 (98%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	h	130/133 (98%)	130 (100%)	0	100	100
37	i	112/113 (99%)	112 (100%)	0	100	100
38	j	101/102 (99%)	100 (99%)	1 (1%)	68	89
39	k	87/92 (95%)	87 (100%)	0	100	100
40	l	90/101 (89%)	90 (100%)	0	100	100
41	m	118/119 (99%)	118 (100%)	0	100	100
42	n	98/102 (96%)	98 (100%)	0	100	100
43	o	51/52 (98%)	51 (100%)	0	100	100
44	p	76/79 (96%)	76 (100%)	0	100	100
45	q	77/81 (95%)	77 (100%)	0	100	100
46	r	75/81 (93%)	75 (100%)	0	100	100
47	s	57/67 (85%)	57 (100%)	0	100	100
48	t	70/79 (89%)	70 (100%)	0	100	100
49	u	61/64 (95%)	61 (100%)	0	100	100
52	F	109/183 (60%)	109 (100%)	0	100	100
53	3	51/79 (65%)	51 (100%)	0	100	100
All	All	4998/5317 (94%)	4996 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	G	156	ARG
38	j	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	15	ASN
1	0	146	HIS
1	0	182	HIS
2	1	48	GLN
6	6	26	ASN
11	G	53	HIS
11	G	177	ASN
12	H	128	GLN

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Mol	Chain	Res	Type
13	I	82	GLN
14	J	161	ASN
15	K	106	ASN
16	M	145	ASN
21	R	32	ASN
23	T	29	HIS
23	T	41	ASN
25	V	102	ASN
31	c	108	GLN
32	d	6	HIS
32	d	99	HIS
34	f	8	HIS
35	g	36	ASN
36	h	153	HIS
38	j	75	GLN
41	m	5	ASN
42	n	91	HIS
43	o	38	HIS
44	p	5	GLN
46	r	53	ASN
49	u	21	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	113/116 (97%)	25 (22%)	3 (2%)
30	a	1513/1558 (97%)	271 (17%)	0
50	D	73/77 (94%)	12 (16%)	1 (1%)
51	b	11/20 (55%)	1 (9%)	0
9	A	2903/2912 (99%)	560 (19%)	39 (1%)
All	All	4613/4683 (98%)	869 (18%)	43 (0%)

All (869) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	8	U
9	A	10	A
9	A	15	G
9	A	28	A
9	A	34	U
9	A	46	C

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Mol	Chain	Res	Type
9	A	51	G
9	A	55	G
9	A	61	A
9	A	71	A
9	A	75	G
9	A	76	C
9	A	77	U
9	A	78	U
9	A	79	U
9	A	85	G
9	A	86	C
9	A	93	U
9	A	96	G
9	A	101	G
9	A	117	A
9	A	119	U
9	A	130	A
9	A	150	A
9	A	163	U
9	A	164	A
9	A	166	A
9	A	167	U
9	A	173	A
9	A	177	G
9	A	181	U
9	A	182	A
9	A	184	A
9	A	186	G
9	A	187	C
9	A	198	A
9	A	199	A
9	A	201	A
9	A	206	A
9	A	215	A
9	A	218	A
9	A	223	A
9	A	225	A
9	A	228	A
9	A	230	A
9	A	231	U
9	A	232	U
9	A	233	C

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Mol	Chain	Res	Type
9	A	235	A
9	A	247	G
9	A	250	G
9	A	251	C
9	A	252	G
9	A	257	A
9	A	263	G
9	A	265	A
9	A	266	G
9	A	267	A
9	A	268	G
9	A	282	G
9	A	289	U
9	A	290	G
9	A	298	U
9	A	299	G
9	A	301	A
9	A	309	G
9	A	311	U
9	A	312	A
9	A	317	A
9	A	318	G
9	A	320	C
9	A	321	U
9	A	322	G
9	A	331	G
9	A	347	A
9	A	352	C
9	A	353	G
9	A	365	G
9	A	366	A
9	A	385	G
9	A	398	A
9	A	403	G
9	A	404	A
9	A	410	A
9	A	411	G
9	A	419	G
9	A	422	C
9	A	425	G
9	A	426	A
9	A	434	C

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Mol	Chain	Res	Type
9	A	442	U
9	A	445	G
9	A	450	G
9	A	459	G
9	A	463	G
9	A	474	C
9	A	475	C
9	A	479	G
9	A	490	U
9	A	494	C
9	A	516	A
9	A	520	G
9	A	521	C
9	A	529	A
9	A	543	A
9	A	545	A
9	A	546	U
9	A	547	C
9	A	548	C
9	A	565	C
9	A	566	A
9	A	568	C
9	A	569	A
9	A	570	A
9	A	571	G
9	A	584	A
9	A	585	A
9	A	586	U
9	A	587	G
9	A	598	U
9	A	599	G
9	A	609	G
9	A	611	A
9	A	622	A
9	A	624	U
9	A	628	G
9	A	639	A
9	A	640	G
9	A	641	G
9	A	651	A
9	A	665	A
9	A	675	A

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Mol	Chain	Res	Type
9	A	683	U
9	A	684	A
9	A	689	G
9	A	692	U
9	A	693	G
9	A	711	C
9	A	716	A
9	A	725	U
9	A	769	A
9	A	784	G
9	A	786	U
9	A	787	G
9	A	796	G
9	A	801	U
9	A	803	A
9	A	804	G
9	A	814	G
9	A	821	A
9	A	823	U
9	A	824	U
9	A	829	A
9	A	830	C
9	A	831	G
9	A	839	A
9	A	844	G
9	A	851	C
9	A	858	A
9	A	866	U
9	A	885	U
9	A	899	G
9	A	906	A
9	A	922	G
9	A	926	A
9	A	928	C
9	A	929	U
9	A	930	C
9	A	931	G
9	A	933	G
9	A	936	A
9	A	947	A
9	A	950	A
9	A	952	C

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Mol	Chain	Res	Type
9	A	954	C
9	A	957	A
9	A	965	U
9	A	970	U
9	A	972	U
9	A	973	A
9	A	980	A
9	A	983	C
9	A	984	A
9	A	985	G
9	A	992	A
9	A	996	A
9	A	998	A
9	A	1000	G
9	A	1013	A
9	A	1021	C
9	A	1022	A
9	A	1024	C
9	A	1035	A
9	A	1051	U
9	A	1052	A
9	A	1056	G
9	A	1061	G
9	A	1062	U
9	A	1064	G
9	A	1065	A
9	A	1066	A
9	A	1067	A
9	A	1072	U
9	A	1086	G
9	A	1101	G
9	A	1109	A
9	A	1110	G
9	A	1115	C
9	A	1122	U
9	A	1123	A
9	A	1124	A
9	A	1126	G
9	A	1127	A
9	A	1130	G
9	A	1151	G
9	A	1155	C

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Mol	Chain	Res	Type
9	A	1158	U
9	A	1165	A
9	A	1166	A
9	A	1167	A
9	A	1169	U
9	A	1171	U
9	A	1172	A
9	A	1174	C
9	A	1175	G
9	A	1181	A
9	A	1182	A
9	A	1188	U
9	A	1196	G
9	A	1212	U
9	A	1213	U
9	A	1215	G
9	A	1221	G
9	A	1231	A
9	A	1240	A
9	A	1241	G
9	A	1244	C
9	A	1245	G
9	A	1248	G
9	A	1256	A
9	A	1265	A
9	A	1267	G
9	A	1274	G
9	A	1284	G
9	A	1286	G
9	A	1289	A
9	A	1292	G
9	A	1302	G
9	A	1307	G
9	A	1308	A
9	A	1311	G
9	A	1315	G
9	A	1335	U
9	A	1336	A
9	A	1347	U
9	A	1348	U
9	A	1360	C
9	A	1364	U

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Mol	Chain	Res	Type
9	A	1373	G
9	A	1376	U
9	A	1380	C
9	A	1383	G
9	A	1384	A
9	A	1385	C
9	A	1387	U
9	A	1400	A
9	A	1414	U
9	A	1419	A
9	A	1420	A
9	A	1421	C
9	A	1422	A
9	A	1423	G
9	A	1424	G
9	A	1427	G
9	A	1430	A
9	A	1431	U
9	A	1451	G
9	A	1454	U
9	A	1455	G
9	A	1457	G
9	A	1460	A
9	A	1461	U
9	A	1462	G
9	A	1468	A
9	A	1469	C
9	A	1470	G
9	A	1475	A
9	A	1480	A
9	A	1484	A
9	A	1486	U
9	A	1494	A
9	A	1495	U
9	A	1496	U
9	A	1497	G
9	A	1502	U
9	A	1503	G
9	A	1509	C
9	A	1511	A
9	A	1520	G
9	A	1523	U

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Mol	Chain	Res	Type
9	A	1524	U
9	A	1526	A
9	A	1530	G
9	A	1531	A
9	A	1534	U
9	A	1535	A
9	A	1537	A
9	A	1538	U
9	A	1543	U
9	A	1546	U
9	A	1551	A
9	A	1553	G
9	A	1555	A
9	A	1562	G
9	A	1565	A
9	A	1567	G
9	A	1569	G
9	A	1572	G
9	A	1575	A
9	A	1576	A
9	A	1579	A
9	A	1580	A
9	A	1581	U
9	A	1582	A
9	A	1583	G
9	A	1584	U
9	A	1599	C
9	A	1600	G
9	A	1604	C
9	A	1614	A
9	A	1618	G
9	A	1623	U
9	A	1627	G
9	A	1629	G
9	A	1630	A
9	A	1649	U
9	A	1650	A
9	A	1652	A
9	A	1658	A
9	A	1677	A
9	A	1688	A
9	A	1689	G

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Mol	Chain	Res	Type
9	A	1690	C
9	A	1694	C
9	A	1704	U
9	A	1705	U
9	A	1709	G
9	A	1710	A
9	A	1714	C
9	A	1716	G
9	A	1742	A
9	A	1745	G
9	A	1753	A
9	A	1755	U
9	A	1756	U
9	A	1757	C
9	A	1758	G
9	A	1759	G
9	A	1766	G
9	A	1769	G
9	A	1770	U
9	A	1775	A
9	A	1776	G
9	A	1777	G
9	A	1786	A
9	A	1798	A
9	A	1799	A
9	A	1804	A
9	A	1812	G
9	A	1813	C
9	A	1821	U
9	A	1823	A
9	A	1828	A
9	A	1829	A
9	A	1830	G
9	A	1842	A
9	A	1861	A
9	A	1867	A
9	A	1869	A
9	A	1871	G
9	A	1882	U
9	A	1883	U
9	A	1884	C
9	A	1896	G

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Mol	Chain	Res	Type
9	A	1918	C
9	A	1919	G
9	A	1923	G
9	A	1927	C
9	A	1929	A
9	A	1940	A
9	A	1942	G
9	A	1943	G
9	A	1949	A
9	A	1950	A
9	A	1951	A
9	A	1953	U
9	A	1954	C
9	A	1968	U
9	A	1973	A
9	A	1976	C
9	A	1977	G
9	A	1978	C
9	A	1979	A
9	A	1980	C
9	A	1983	A
9	A	1984	A
9	A	1985	G
9	A	2004	U
9	A	2006	U
9	A	2010	A
9	A	2035	U
9	A	2044	A
9	A	2045	G
9	A	2046	A
9	A	2056	C
9	A	2062	A
9	A	2068	C
9	A	2069	G
9	A	2072	A
9	A	2073	A
9	A	2074	G
9	A	2075	A
9	A	2082	G
9	A	2093	G
9	A	2107	A
9	A	2108	G

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Mol	Chain	Res	Type
9	A	2112	U
9	A	2113	U
9	A	2117	C
9	A	2121	A
9	A	2124	U
9	A	2129	G
9	A	2130	A
9	A	2139	A
9	A	2145	U
9	A	2146	G
9	A	2170	G
9	A	2172	G
9	A	2173	G
9	A	2185	U
9	A	2191	C
9	A	2196	U
9	A	2203	A
9	A	2207	C
9	A	2211	A
9	A	2216	G
9	A	2217	C
9	A	2224	A
9	A	2230	G
9	A	2238	A
9	A	2251	G
9	A	2252	G
9	A	2259	G
9	A	2262	U
9	A	2279	A
9	A	2281	A
9	A	2291	A
9	A	2292	G
9	A	2296	C
9	A	2300	A
9	A	2301	A
9	A	2302	G
9	A	2318	U
9	A	2320	G
9	A	2322	A
9	A	2331	G
9	A	2333	A
9	A	2334	G

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Mol	Chain	Res	Type
9	A	2335	A
9	A	2340	A
9	A	2347	G
9	A	2348	A
9	A	2360	C
9	A	2363	C
9	A	2367	A
9	A	2371	A
9	A	2374	A
9	A	2396	G
9	A	2399	U
9	A	2404	G
9	A	2409	G
9	A	2415	U
9	A	2420	A
9	A	2436	U
9	A	2438	A
9	A	2439	A
9	A	2442	G
9	A	2443	A
9	A	2447	A
9	A	2454	C
9	A	2458	G
9	A	2461	A
9	A	2464	A
9	A	2481	A
9	A	2489	A
9	A	2491	A
9	A	2493	C
9	A	2507	G
9	A	2515	G
9	A	2519	U
9	A	2526	G
9	A	2531	A
9	A	2533	C
9	A	2542	G
9	A	2548	G
9	A	2567	U
9	A	2577	A
9	A	2579	A
9	A	2580	G
9	A	2586	C

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Mol	Chain	Res	Type
9	A	2591	G
9	A	2597	U
9	A	2598	U
9	A	2615	A
9	A	2622	U
9	A	2623	C
9	A	2626	U
9	A	2628	U
9	A	2642	U
9	A	2645	A
9	A	2659	C
9	A	2695	G
9	A	2698	G
9	A	2702	U
9	A	2727	G
9	A	2731	G
9	A	2746	A
9	A	2749	G
9	A	2764	G
9	A	2770	A
9	A	2778	A
9	A	2790	G
9	A	2791	A
9	A	2792	U
9	A	2802	C
9	A	2804	U
9	A	2808	U
9	A	2809	U
9	A	2810	U
9	A	2811	A
9	A	2812	A
9	A	2813	G
9	A	2816	A
9	A	2843	A
9	A	2853	G
9	A	2859	G
9	A	2860	A
9	A	2863	G
9	A	2871	U
9	A	2877	G
9	A	2882	G
9	A	2884	C

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Mol	Chain	Res	Type
9	A	2890	C
9	A	2893	A
9	A	2896	G
9	A	2902	G
9	A	2903	G
9	A	2909	A
9	A	2910	C
9	A	2911	C
10	B	10	G
10	B	11	A
10	B	12	U
10	B	14	G
10	B	23	A
10	B	28	C
10	B	32	U
10	B	34	C
10	B	35	C
10	B	39	G
10	B	40	C
10	B	42	G
10	B	49	G
10	B	50	A
10	B	55	A
10	B	64	A
10	B	65	G
10	B	82	G
10	B	87	U
10	B	88	C
10	B	97	A
10	B	101	U
10	B	107	G
10	B	108	U
10	B	110	G
30	a	10	A
30	a	11	G
30	a	24	G
30	a	33	G
30	a	34	A
30	a	41	G
30	a	46	G
30	a	49	C
30	a	50	C

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Mol	Chain	Res	Type
30	a	51	U
30	a	53	A
30	a	56	C
30	a	57	A
30	a	116	G
30	a	117	A
30	a	118	G
30	a	132	A
30	a	136	A
30	a	137	C
30	a	138	A
30	a	146	A
30	a	147	A
30	a	158	A
30	a	161	G
30	a	166	A
30	a	172	C
30	a	175	G
30	a	177	A
30	a	180	C
30	a	181	A
30	a	182	G
30	a	190	U
30	a	199	A
30	a	200	C
30	a	207	U
30	a	213	A
30	a	215	G
30	a	226	G
30	a	227	A
30	a	230	G
30	a	266	U
30	a	267	G
30	a	270	U
30	a	271	U
30	a	273	G
30	a	277	G
30	a	279	U
30	a	292	G
30	a	293	C
30	a	315	G
30	a	332	A

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Mol	Chain	Res	Type
30	a	347	A
30	a	354	C
30	a	355	A
30	a	358	G
30	a	370	A
30	a	373	G
30	a	378	C
30	a	380	G
30	a	381	C
30	a	389	A
30	a	390	A
30	a	391	U
30	a	393	U
30	a	398	C
30	a	399	A
30	a	414	G
30	a	417	C
30	a	418	G
30	a	423	A
30	a	430	G
30	a	432	G
30	a	437	A
30	a	438	A
30	a	439	G
30	a	447	U
30	a	448	C
30	a	450	G
30	a	453	C
30	a	454	G
30	a	455	U
30	a	474	A
30	a	477	A
30	a	478	A
30	a	479	C
30	a	485	C
30	a	488	U
30	a	489	A
30	a	490	G
30	a	491	U
30	a	511	G
30	a	512	U
30	a	521	A

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Mol	Chain	Res	Type
30	a	522	G
30	a	523	A
30	a	535	A
30	a	537	C
30	a	544	C
30	a	547	G
30	a	553	G
30	a	556	G
30	a	557	U
30	a	558	A
30	a	573	A
30	a	578	U
30	a	585	A
30	a	590	U
30	a	598	A
30	a	599	A
30	a	602	C
30	a	603	G
30	a	605	G
30	a	622	A
30	a	658	G
30	a	659	U
30	a	660	C
30	a	668	A
30	a	679	U
30	a	687	G
30	a	691	A
30	a	709	G
30	a	720	A
30	a	721	A
30	a	728	A
30	a	730	A
30	a	736	G
30	a	747	A
30	a	749	U
30	a	750	G
30	a	755	A
30	a	759	G
30	a	760	G
30	a	772	G
30	a	775	A
30	a	781	G

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Mol	Chain	Res	Type
30	a	813	A
30	a	819	U
30	a	820	A
30	a	836	C
30	a	843	C
30	a	846	U
30	a	855	A
30	a	858	G
30	a	862	G
30	a	866	G
30	a	873	C
30	a	899	A
30	a	903	A
30	a	916	A
30	a	941	A
30	a	953	G
30	a	954	G
30	a	961	C
30	a	962	A
30	a	966	G
30	a	972	G
30	a	983	U
30	a	987	U
30	a	993	G
30	a	995	A
30	a	996	A
30	a	998	G
30	a	1002	A
30	a	1003	G
30	a	1004	A
30	a	1009	U
30	a	1016	U
30	a	1019	U
30	a	1020	G
30	a	1023	A
30	a	1028	U
30	a	1029	U
30	a	1030	G
30	a	1031	A
30	a	1034	A
30	a	1036	U
30	a	1039	A

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Mol	Chain	Res	Type
30	a	1040	G
30	a	1045	A
30	a	1047	A
30	a	1050	U
30	a	1052	U
30	a	1053	C
30	a	1063	A
30	a	1064	C
30	a	1066	A
30	a	1067	A
30	a	1070	G
30	a	1073	A
30	a	1075	G
30	a	1077	G
30	a	1078	G
30	a	1081	C
30	a	1083	U
30	a	1092	U
30	a	1093	C
30	a	1112	U
30	a	1119	A
30	a	1121	G
30	a	1122	U
30	a	1127	C
30	a	1128	A
30	a	1129	A
30	a	1131	G
30	a	1135	G
30	a	1159	C
30	a	1165	G
30	a	1166	U
30	a	1171	C
30	a	1172	A
30	a	1183	A
30	a	1185	U
30	a	1187	C
30	a	1193	A
30	a	1194	C
30	a	1210	G
30	a	1222	A
30	a	1223	A
30	a	1228	U

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Mol	Chain	Res	Type
30	a	1238	U
30	a	1239	A
30	a	1253	A
30	a	1254	C
30	a	1262	A
30	a	1283	C
30	a	1286	U
30	a	1306	A
30	a	1307	U
30	a	1319	U
30	a	1325	A
30	a	1326	G
30	a	1328	U
30	a	1331	G
30	a	1340	C
30	a	1343	C
30	a	1344	A
30	a	1348	C
30	a	1361	C
30	a	1362	C
30	a	1379	G
30	a	1386	A
30	a	1407	U
30	a	1415	C
30	a	1420	A
30	a	1423	C
30	a	1424	A
30	a	1428	C
30	a	1445	G
30	a	1448	U
30	a	1452	A
30	a	1468	A
30	a	1472	A
30	a	1478	U
30	a	1479	U
30	a	1480	U
30	a	1481	G
30	a	1502	G
30	a	1514	G
30	a	1517	U
30	a	1519	A
30	a	1524	G

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Mol	Chain	Res	Type
30	a	1530	A
30	a	1533	U
30	a	1534	A
30	a	1544	G
30	a	1546	A
30	a	1556	G
30	a	1557	G
30	a	1558	A
30	a	1561	A
30	a	1564	U
50	D	4	G
50	D	8	U
50	D	14	A
50	D	21	U
50	D	22	A
50	D	23	G
50	D	44	A
50	D	47	G
50	D	48	U
50	D	65	G
50	D	72	C
50	D	73	A
51	b	16	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	92	G
9	A	174	U
9	A	199	A
9	A	231	U
9	A	251	C
9	A	288	U
9	A	433	C
9	A	520	G
9	A	658	G
9	A	774	A
9	A	802	G
9	A	823	U
9	A	982	U
9	A	1033	C
9	A	1239	A

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Mol	Chain	Res	Type
9	A	1240	A
9	A	1301	A
9	A	1335	U
9	A	1347	U
9	A	1450	U
9	A	1525	G
9	A	1530	G
9	A	1536	A
9	A	1561	U
9	A	1583	G
9	A	1693	G
9	A	1797	A
9	A	1812	G
9	A	1828	A
9	A	1866	A
9	A	1868	G
9	A	1926	A
9	A	2111	U
9	A	2300	A
9	A	2419	C
9	A	2438	A
9	A	2789	A
9	A	2808	U
9	A	2810	U
10	B	31	G
10	B	48	A
10	B	49	G
50	D	22	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 185 ligands modelled in this entry, 179 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	PUT	A	3139	-	5,5,5	0.21	0	4,4,4	0.47	0
54	ATP	0	602	55	32,33,33	0.70	2 (6%)	48,52,52	0.29	0
54	ATP	0	601	55	32,33,33	0.59	1 (3%)	48,52,52	0.34	0
58	PUT	A	3138	-	5,5,5	0.24	0	4,4,4	0.35	0
58	PUT	a	1633	-	5,5,5	0.23	0	4,4,4	0.41	0
58	PUT	a	1634	-	5,5,5	0.19	0	4,4,4	0.46	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
58	PUT	A	3139	-	-	1/3/3/3	-
54	ATP	0	602	55	-	4/22/38/38	0/3/3/3
54	ATP	0	601	55	-	3/22/38/38	0/3/3/3
58	PUT	A	3138	-	-	1/3/3/3	-
58	PUT	a	1633	-	-	0/3/3/3	-
58	PUT	a	1634	-	-	0/3/3/3	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	0	602	ATP	PB-O3B	-2.35	1.57	1.59
54	0	601	ATP	PB-O3B	-2.25	1.57	1.59
54	0	602	ATP	PA-O3A	-2.25	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	0	602	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
58	A	3138	PUT	C1-C2-C3-C4
54	0	602	ATP	PG-O3B-PB-O2B
54	0	601	ATP	O4'-C4'-C5'-O5'
54	0	602	ATP	PG-O3B-PB-O1B
54	0	601	ATP	PB-O3B-PG-O3G
54	0	602	ATP	PB-O3B-PG-O3G
54	0	601	ATP	C3'-C4'-C5'-O5'
58	A	3139	PUT	C2-C3-C4-N2

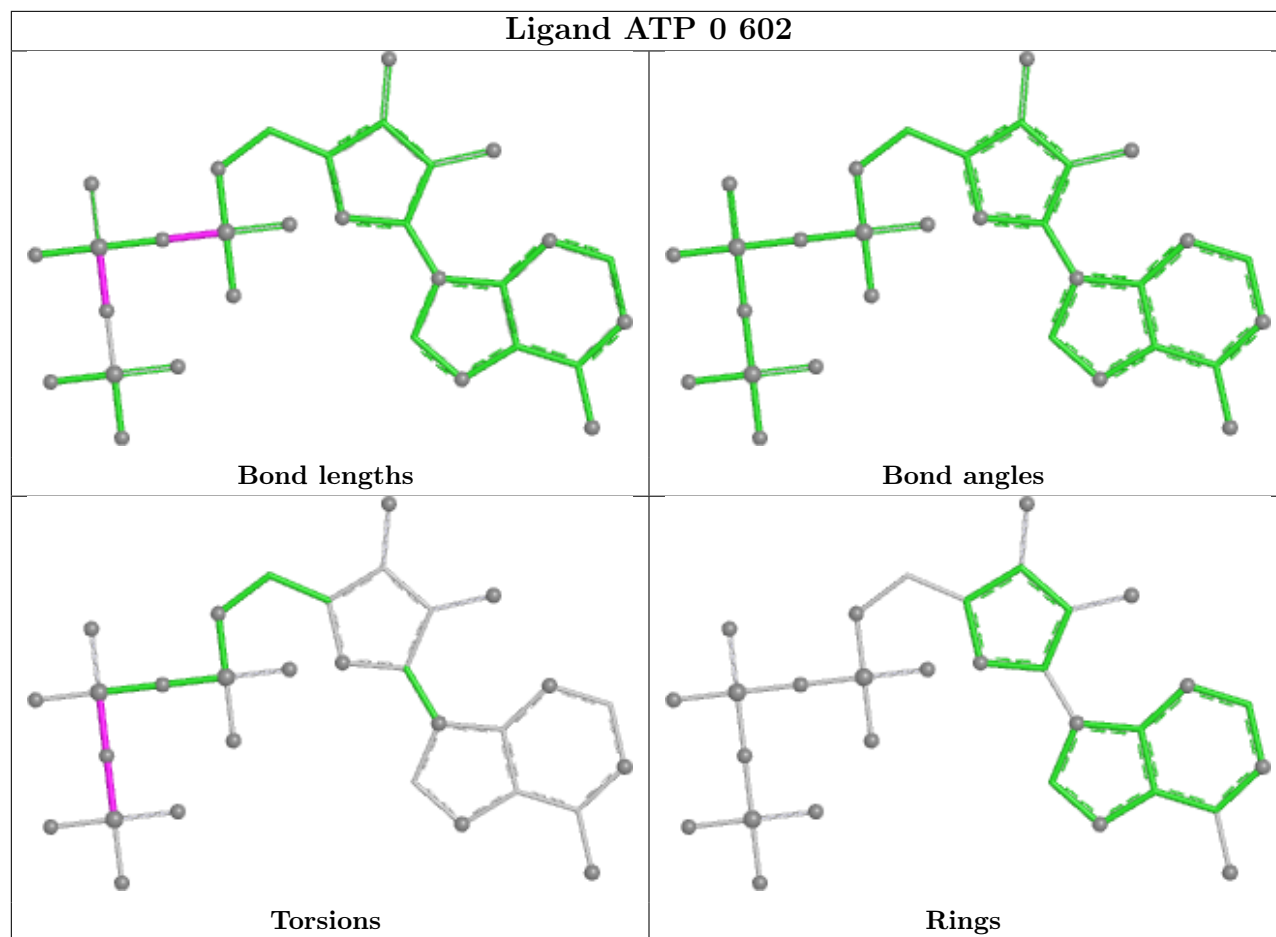
There are no ring outliers.

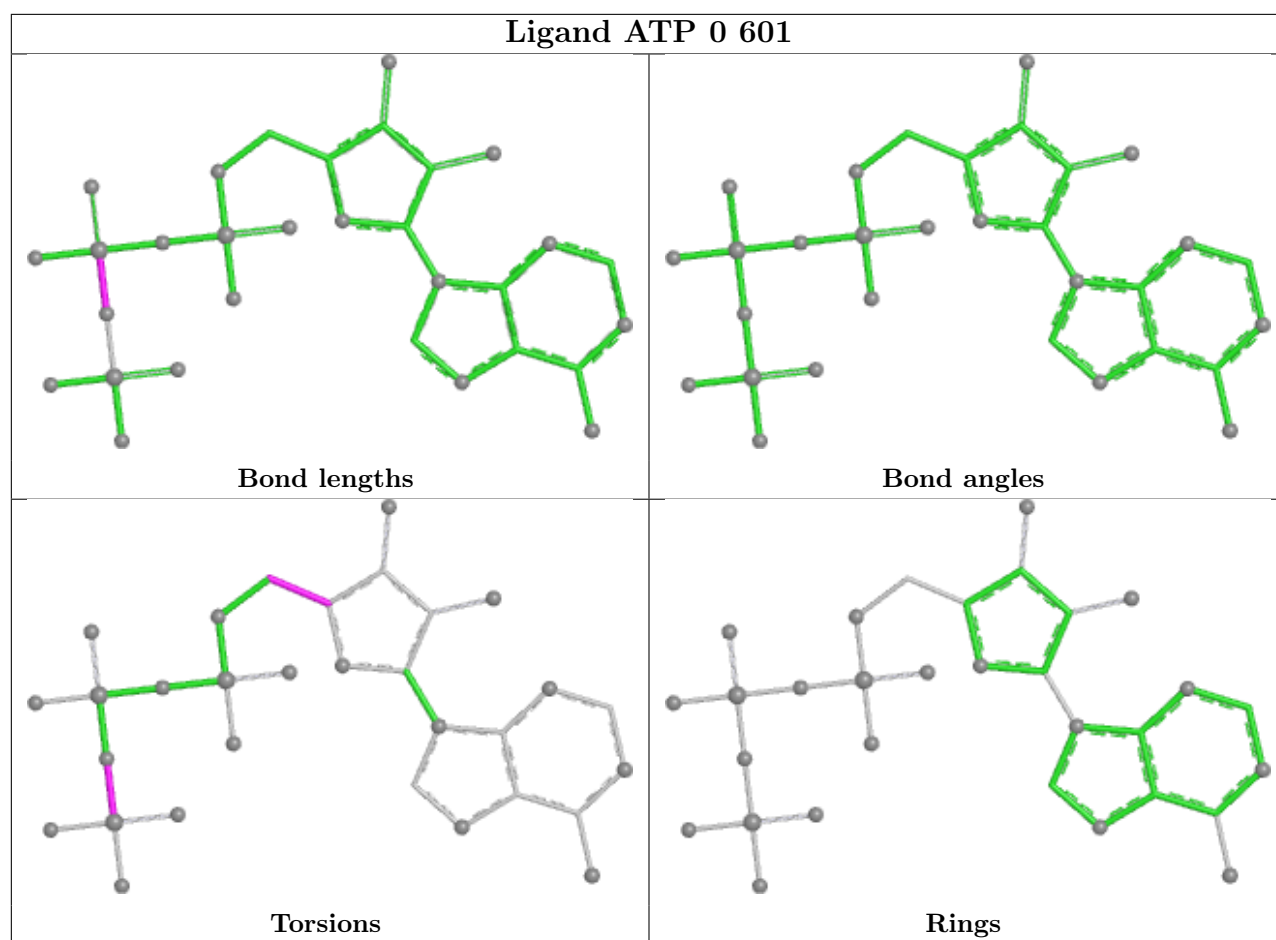
1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	0	601	ATP	6	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.

Ligand ATP 0 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

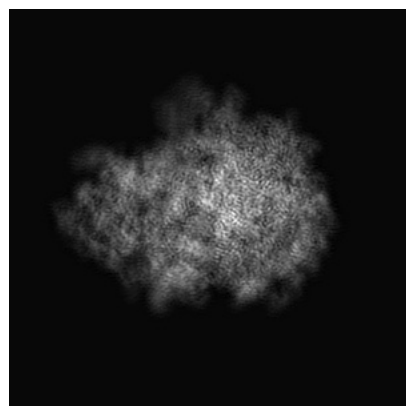
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12331. These allow visual inspection of the internal detail of the map and identification of artifacts.

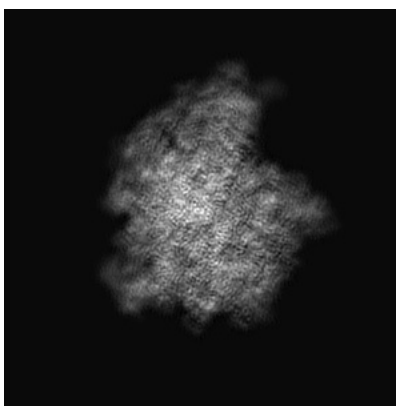
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

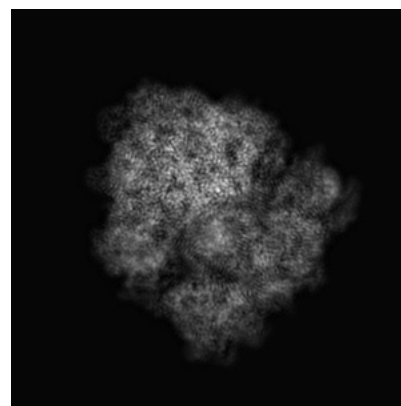
6.1.1 Primary map



X

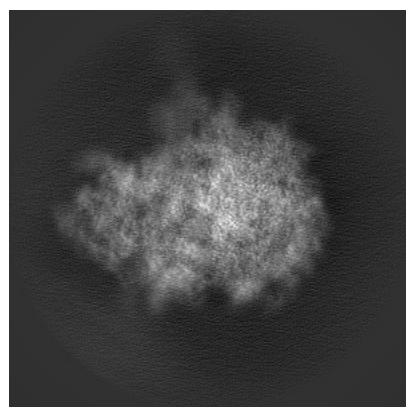


Y

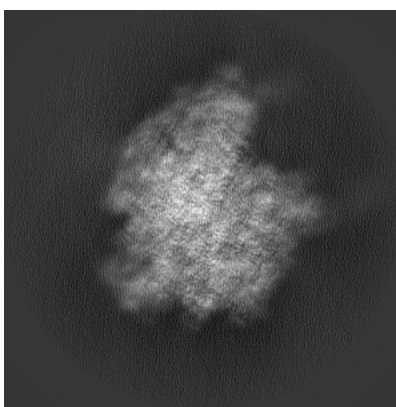


Z

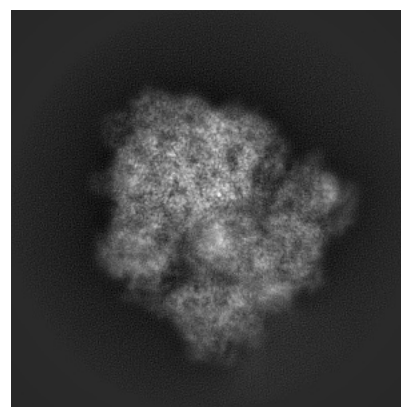
6.1.2 Raw map



X



Y

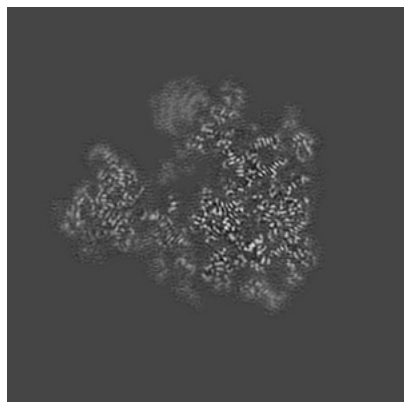


Z

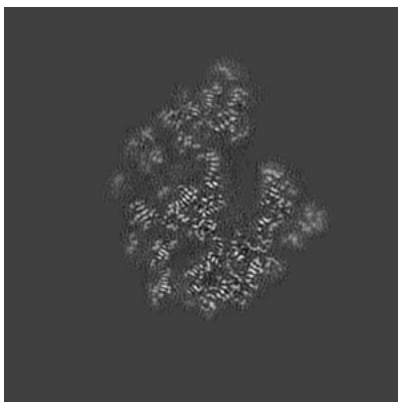
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

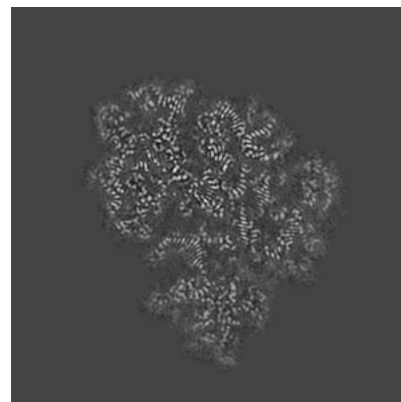
6.2.1 Primary map



X Index: 176

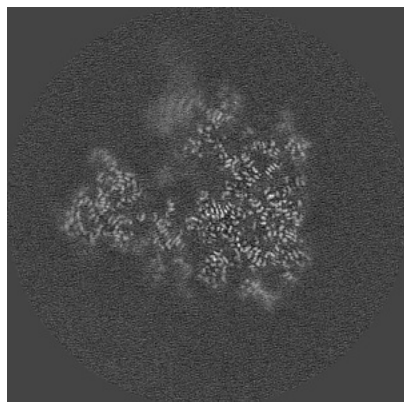


Y Index: 176

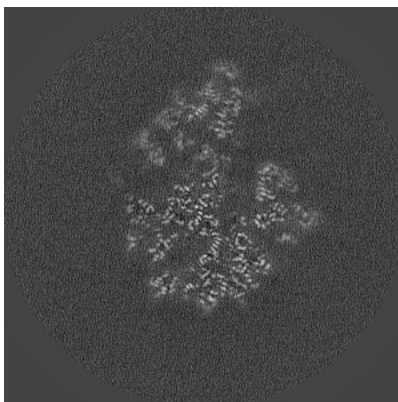


Z Index: 176

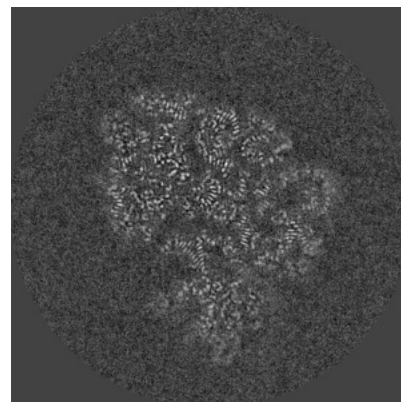
6.2.2 Raw map



X Index: 180



Y Index: 180

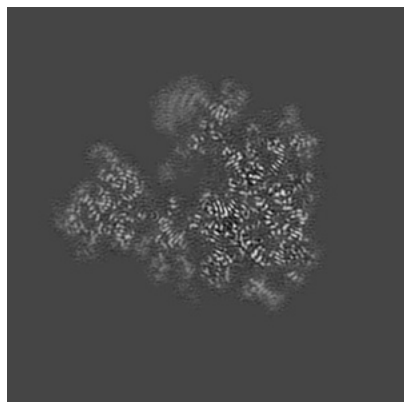


Z Index: 180

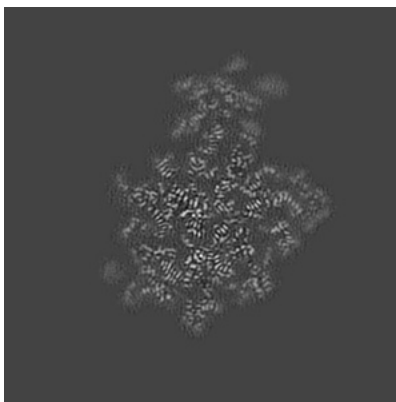
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

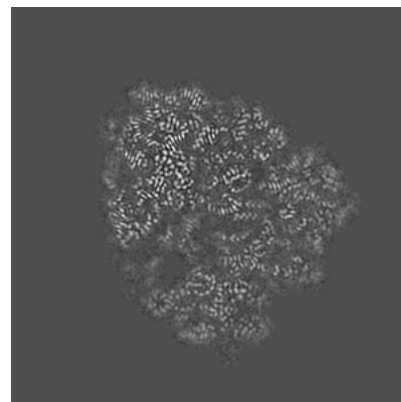
6.3.1 Primary map



X Index: 174

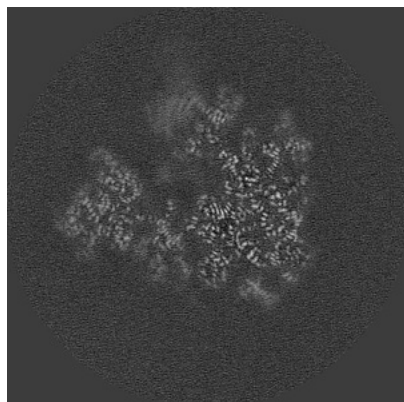


Y Index: 197

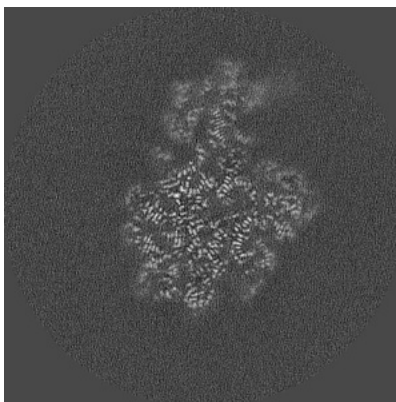


Z Index: 186

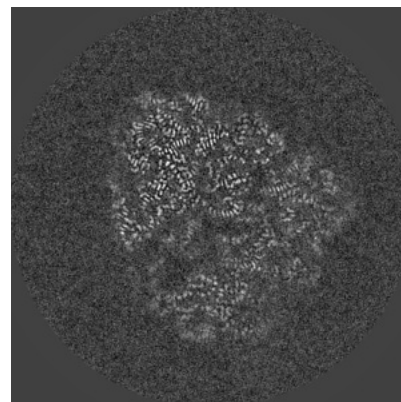
6.3.2 Raw map



X Index: 179



Y Index: 190

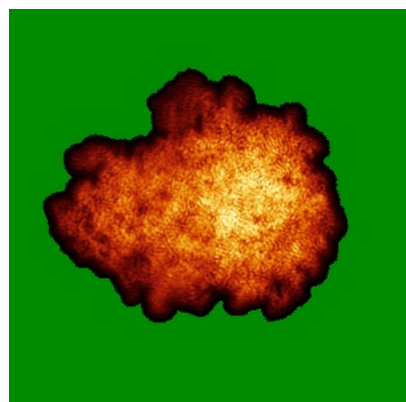


Z Index: 189

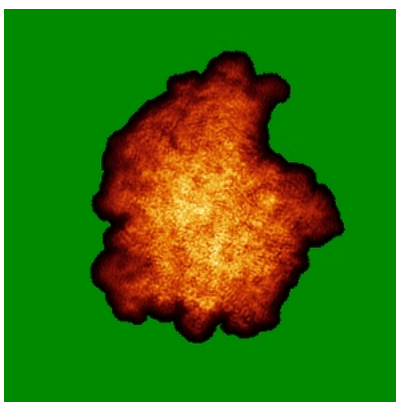
The images above show the largest variance slices of the map in three orthogonal directions.

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

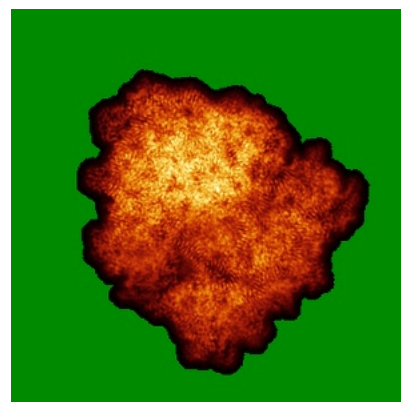
6.4.1 Primary map



X

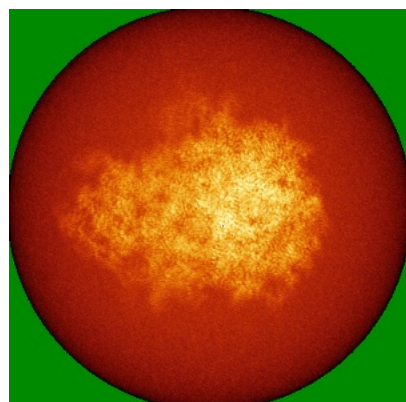


Y

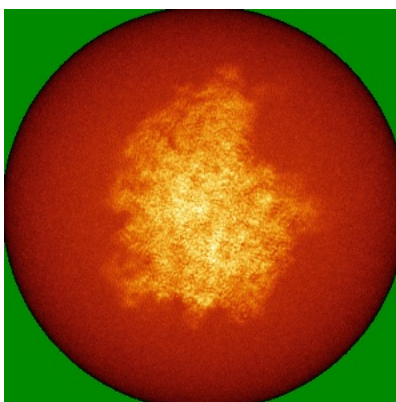


Z

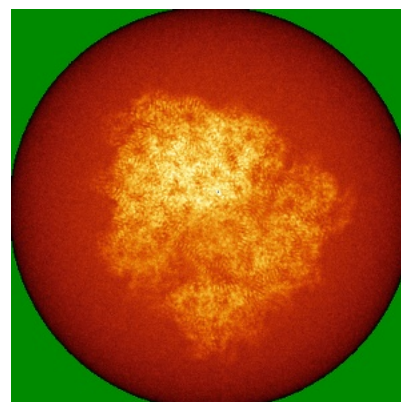
6.4.2 Raw map



X



Y

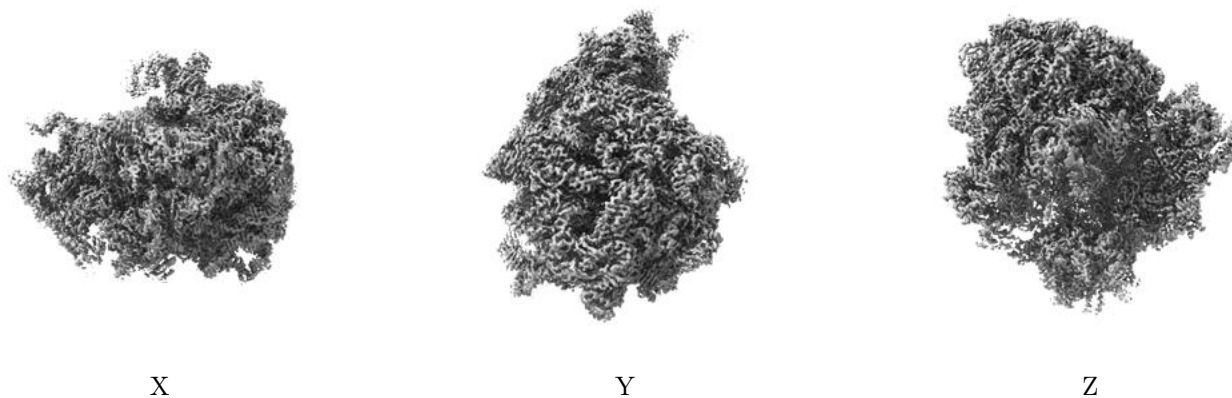


Z

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.

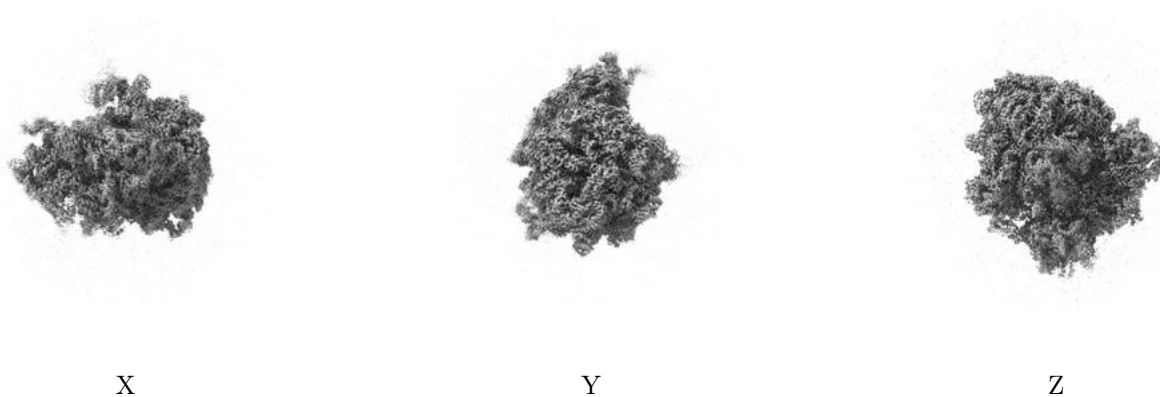
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

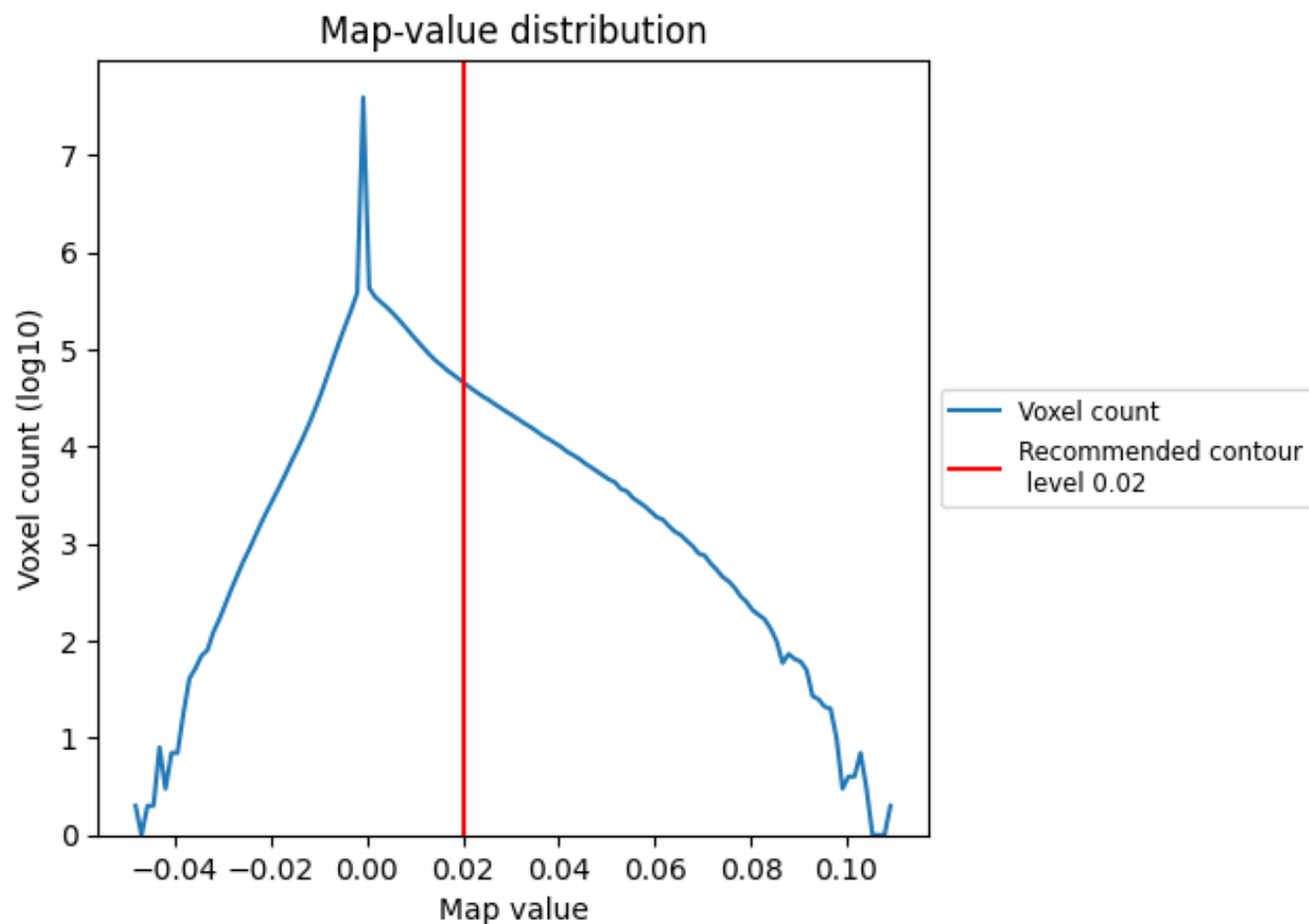
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

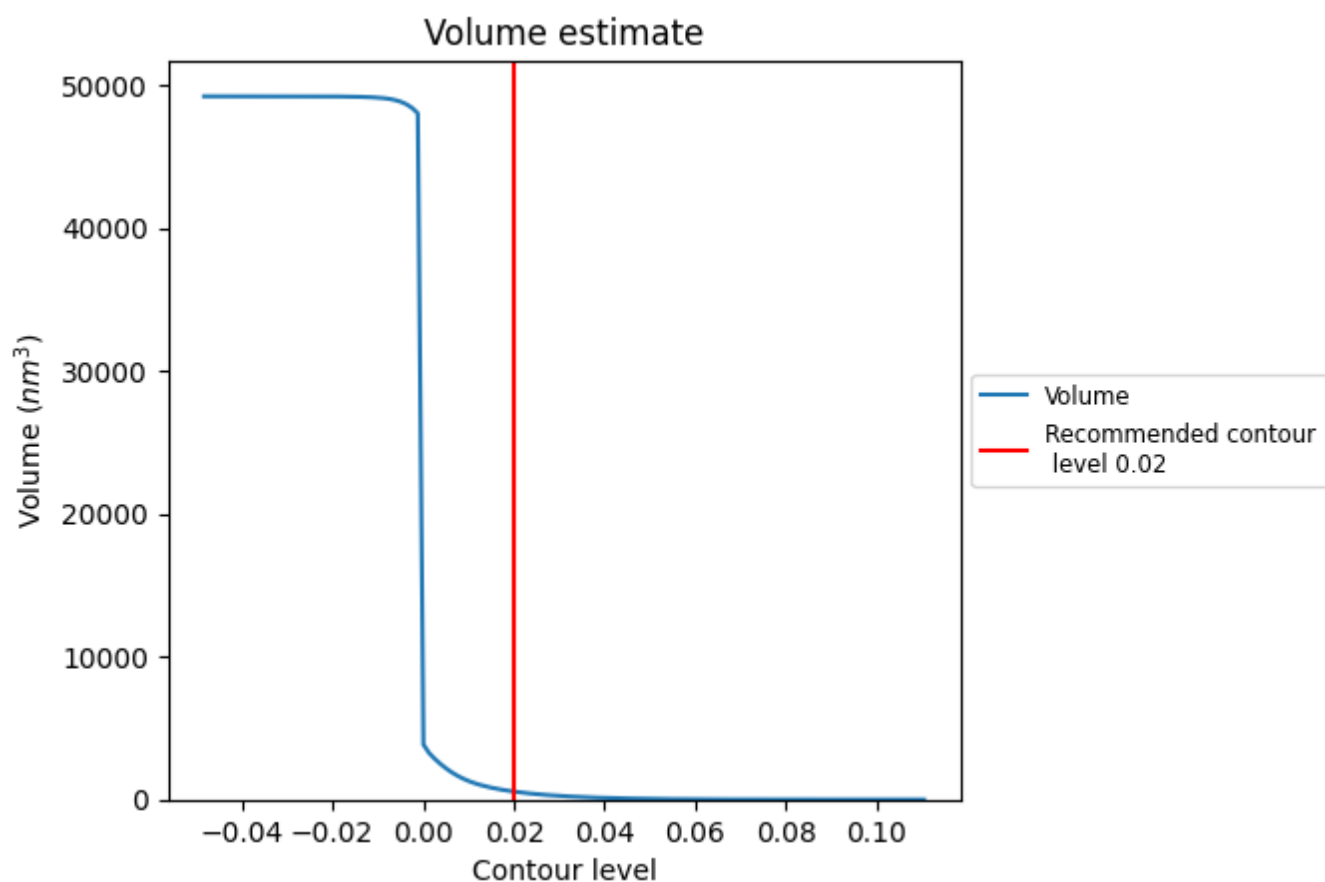
This section contains the results of statistical analysis of the map.

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.

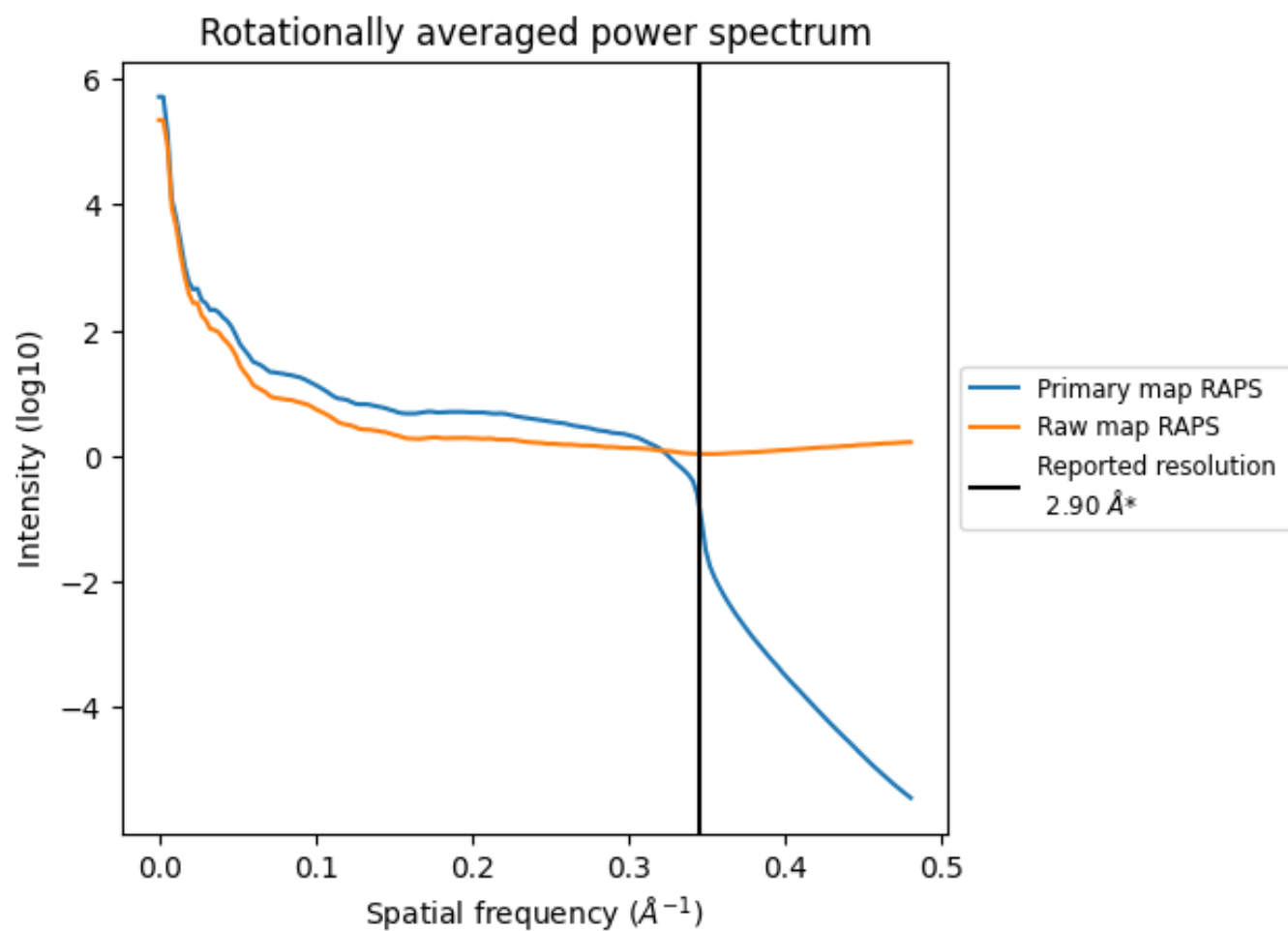
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 560 nm³; this corresponds to an approximate mass of 505 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 ⓘ

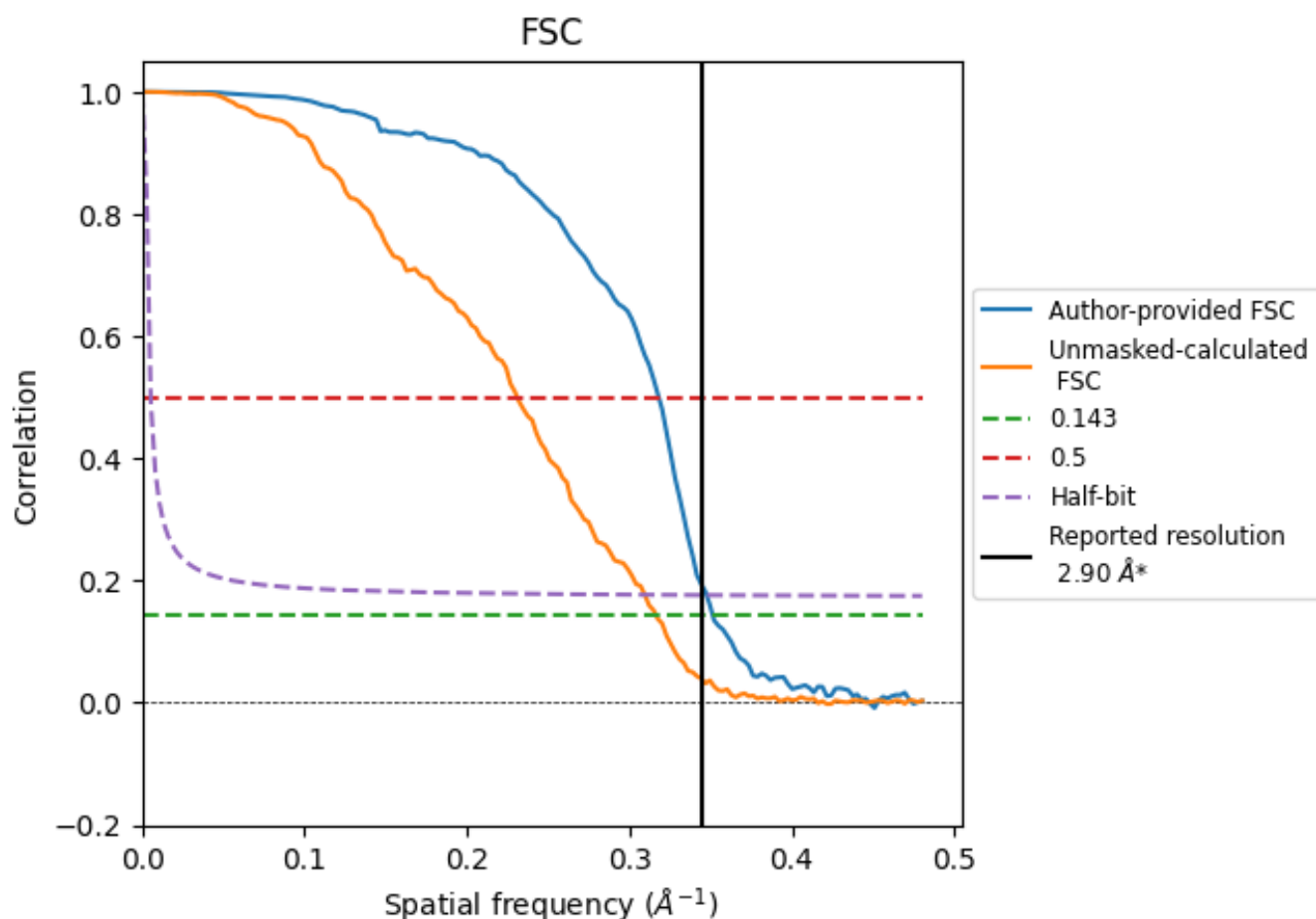


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

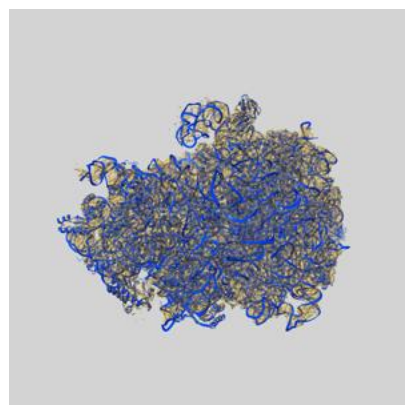
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.85	3.14	2.88
Unmasked-calculated*	3.16	4.33	3.23

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

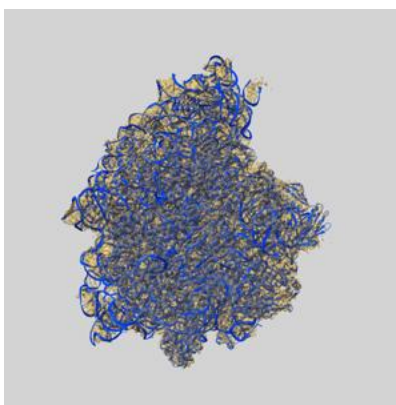
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12331 and PDB model 7NHK. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

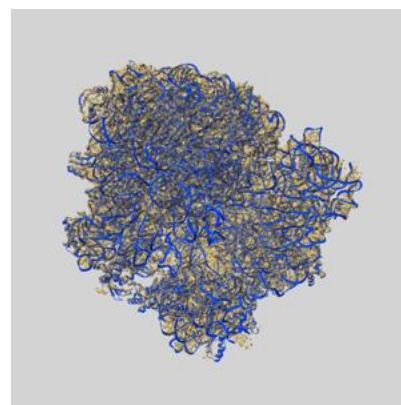
9.1 Map-model overlay [i](#)



X



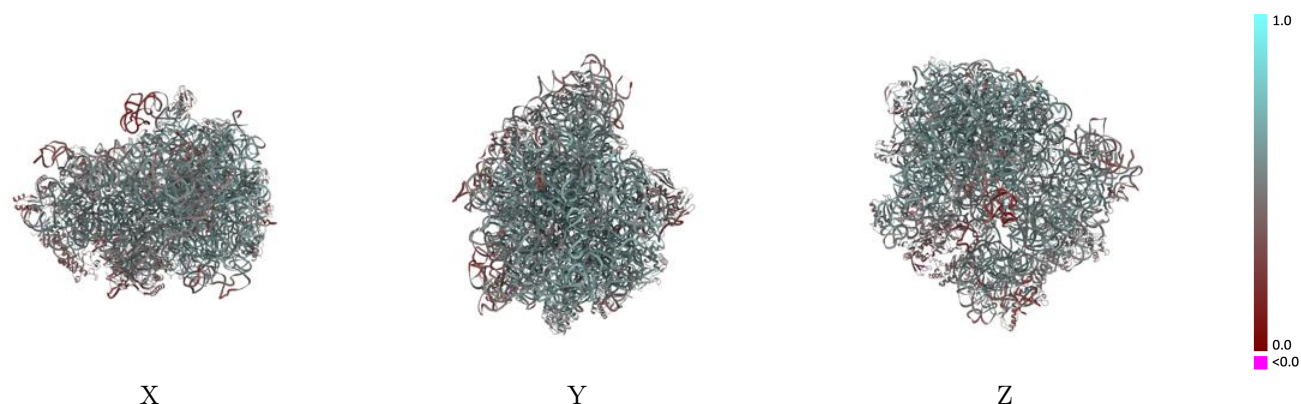
Y



Z

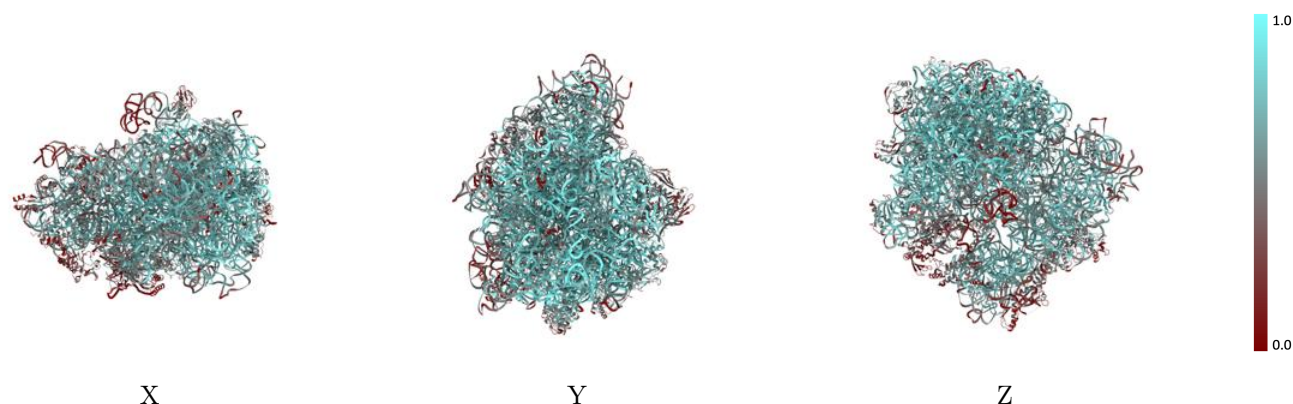
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



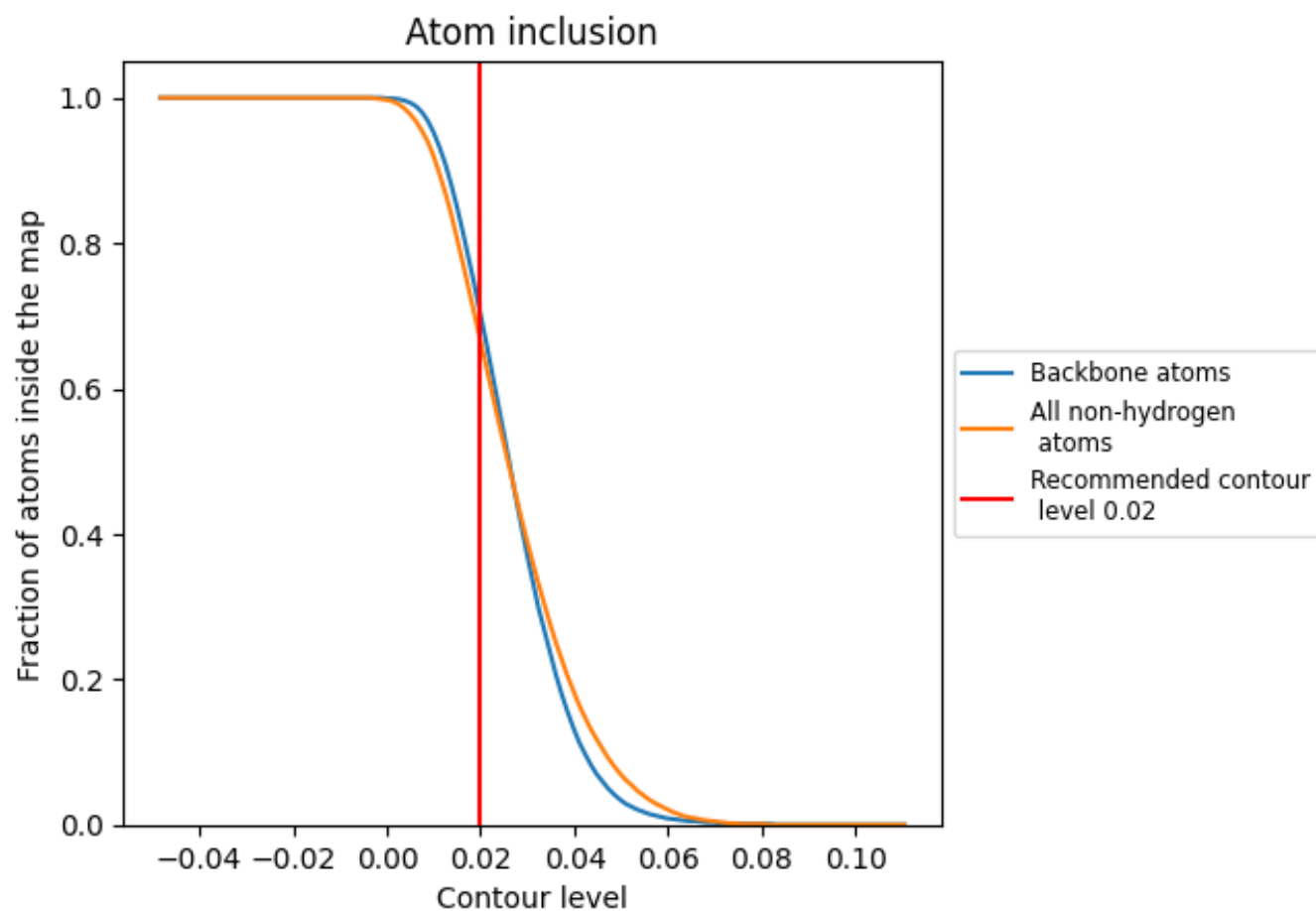
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 66% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6650	 0.5190
0	 0.4790	 0.4870
1	 0.4820	 0.4540
2	 0.5660	 0.5120
3	 0.1780	 0.3520
4	 0.7230	 0.5470
5	 0.6190	 0.4940
6	 0.6790	 0.5650
7	 0.7000	 0.5540
8	 0.6760	 0.5430
A	 0.7760	 0.5490
B	 0.6660	 0.5180
D	 0.6170	 0.5310
F	 0.0090	 0.2090
G	 0.6600	 0.5440
H	 0.6510	 0.5380
I	 0.5920	 0.5100
J	 0.2410	 0.3860
K	 0.3870	 0.4400
M	 0.6330	 0.5320
N	 0.5690	 0.5210
O	 0.5820	 0.5230
P	 0.6500	 0.5200
Q	 0.6300	 0.5130
R	 0.5130	 0.4800
S	 0.5960	 0.5210
T	 0.6870	 0.5450
U	 0.6010	 0.5280
V	 0.6530	 0.5410
W	 0.5560	 0.4980
X	 0.4440	 0.4770
Y	 0.6830	 0.5470
Z	 0.5450	 0.5270
a	 0.7060	 0.5240
b	 0.4770	 0.4650



Continued on next page...

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Chain	Atom inclusion	Q-score
c	 0.2960	 0.4040
d	 0.4690	 0.4680
e	 0.3860	 0.4400
f	 0.4550	 0.4680
g	 0.1820	 0.3860
h	 0.4010	 0.4450
i	 0.4260	 0.4650
j	 0.4590	 0.4730
k	 0.3980	 0.4400
l	 0.3290	 0.4180
m	 0.5530	 0.5240
n	 0.3880	 0.4430
o	 0.6110	 0.5130
p	 0.4130	 0.4270
q	 0.4640	 0.4640
r	 0.4250	 0.4640
s	 0.2610	 0.4180
t	 0.4150	 0.4400
u	 0.4680	 0.4530