



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:12 PM UTC

PDB ID : 7NHL / pdb_00007nhl
EMDB ID : EMD-12332
Title : VgaA-LC, an antibiotic resistance ABCF, in complex with 70S ribosome from *Staphylococcus aureus*
Authors : Crowe-McAuliffe, C.; Murina, V.; Hauryliuk, V.; Wilson, D.N.
Deposited on : 2021-02-10
Resolution : 3.10 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:

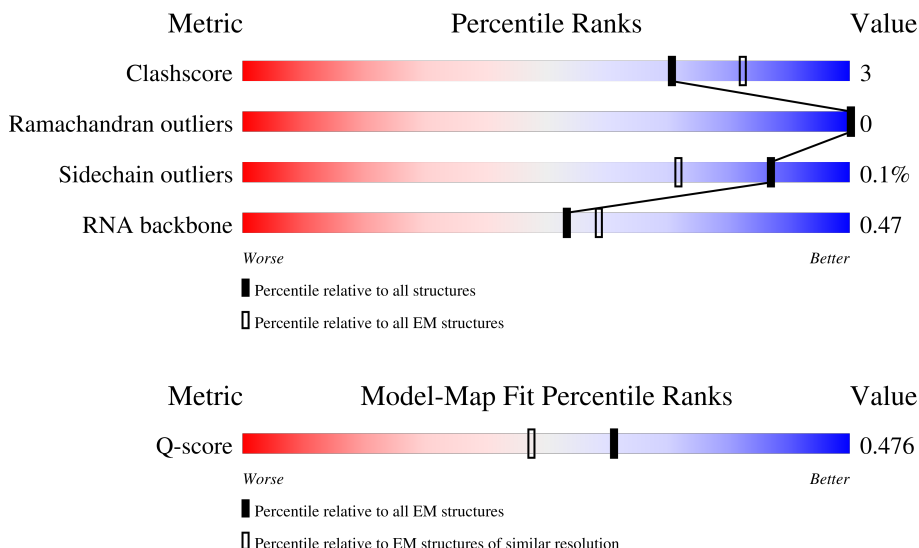
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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	14724 (2.60 - 3.60)

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	546	26% 74% 11% 15%
2	D	76	64% 28% •
3	Z	94	7% 67% 14% 19%

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Mol	Chain	Length	Quality of chain
4	P	144	
5	A	2923	
6	a	1551	
7	B	115	
8	G	277	
9	H	220	
10	I	207	
11	J	179	
12	K	178	
13	M	145	
14	N	122	
15	O	146	
16	Q	122	
17	R	119	
18	S	116	
19	T	118	
20	U	102	
21	V	117	
22	W	91	
23	X	105	
24	Y	217	
25	1	62	
26	2	69	
27	3	59	
28	6	49	

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Mol	Chain	Length	Quality of chain
29	8	66	
30	7	45	
31	d	217	
32	e	200	
33	h	156	
34	k	102	
35	l	129	
36	o	60	
37	p	89	
38	q	91	
39	u	83	
40	9	37	
41	t	92	
42	n	121	
43	j	132	
44	f	166	
45	i	132	
46	s	80	
47	g	98	
48	b	15	
49	m	137	
50	r	87	
51	c	255	
52	4	84	
53	5	57	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145969 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 Lincosamide-streptogramin A resistance protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	465	Total	C	N	O	S	0	0
			3770	2397	659	707	7		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	105	GLN	GLU	engineered mutation	UNP A0SNL9
0	410	GLN	GLU	engineered mutation	UNP A0SNL9
0	523	GLY	-	expression tag	UNP A0SNL9
0	524	GLY	-	expression tag	UNP A0SNL9
0	525	ASP	-	expression tag	UNP A0SNL9
0	526	TYR	-	expression tag	UNP A0SNL9
0	527	LYS	-	expression tag	UNP A0SNL9
0	528	ASP	-	expression tag	UNP A0SNL9
0	529	HIS	-	expression tag	UNP A0SNL9
0	530	ASP	-	expression tag	UNP A0SNL9
0	531	GLY	-	expression tag	UNP A0SNL9
0	532	ASP	-	expression tag	UNP A0SNL9
0	533	TYR	-	expression tag	UNP A0SNL9
0	534	LYS	-	expression tag	UNP A0SNL9
0	535	ASP	-	expression tag	UNP A0SNL9
0	536	HIS	-	expression tag	UNP A0SNL9
0	537	ASP	-	expression tag	UNP A0SNL9
0	538	ILE	-	expression tag	UNP A0SNL9
0	539	ASP	-	expression tag	UNP A0SNL9
0	540	TYR	-	expression tag	UNP A0SNL9
0	541	LYS	-	expression tag	UNP A0SNL9
0	542	ASP	-	expression tag	UNP A0SNL9
0	543	ASP	-	expression tag	UNP A0SNL9
0	544	ASP	-	expression tag	UNP A0SNL9
0	545	ASP	-	expression tag	UNP A0SNL9
0	546	LYS	-	expression tag	UNP A0SNL9

- Molecule 2 is a RNA chain called P-tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	73	Total	C	N	O	P	0	0
			1562	696	284	509	73		

- Molecule 3 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Z	76	Total	C	N	O		0	0
			585	361	114	110			

- Molecule 4 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	135	Total	C	N	O	S	0	0
			1081	693	205	180	3		

- Molecule 5 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2914	Total	C	N	O	P	0	0
			62482	27895	11429	20244	2914		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	1538	Total	C	N	O	P	0	0
			32937	14706	6006	10687	1538		

- Molecule 7 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 8 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	273	Total	C	N	O	S	0	0
			2085	1297	413	370	5		

- Molecule 9 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	216	Total	C	N	O	S	0	0
			1637	1024	301	307	5		

- Molecule 10 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	204	Total	C	N	O	S	0	0
			1564	981	286	295	2		

- Molecule 11 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	175	Total	C	N	O	S	0	0
			1381	876	237	261	7		

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	164	Total	C	N	O	S	0	0
			1284	799	232	250	3		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	142	Total	C	N	O	S	0	0
			1127	704	205	216	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	145	Total	C	N	O	S	0	0
			1090	674	214	201	1		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	118	Total	C	N	O		0	0
			914	569	173	172			

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	114	Total	C	N	O		0	0
			922	580	185	157			

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	101	Total	C	N	O	S	0	0
			793	503	141	148	1		

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	99	Total	C	N	O	S	0	0
			761	480	140	139	2		

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	60	Total	C	N	O	S	0	0
			474	293	103	77	1		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	2	64	Total	C	N	O	0	0
			527	324	99	104		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	3	56	Total	C	N	O	0	0
			436	271	82	83		

- Molecule 28 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	47	Total	C	N	O	S	0	0
			389	232	79	74	4		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	8	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	42	Total	C	N	O	S	0	0
			360	220	88	51	1		

- Molecule 31 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	208	Total	C	N	O	S	0	0
			1638	1032	306	298	2		

- Molecule 32 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 33 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1101	686	208	203	4		

- Molecule 34 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	100	Total	C	N	O	S	0	0
			801	505	147	148	1		

- Molecule 35 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	118	Total	C	N	O	S	0	0
			876	542	166	165	3		

- Molecule 36 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	o	59	Total	C	N	O	S	0	0
			496	314	99	78	5		

- Molecule 37 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	p	87	Total	C	N	O	S	0	0
			733	451	152	129	1		

- Molecule 38 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 39 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 40 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	9	36	Total	C	N	O	S	0	0
			292	184	59	44	5		

- Molecule 41 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	79	Total	C	N	O	S	0	0
			646	416	116	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	116	Total	C	N	O	S	0	0
			922	566	183	172	1		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	127	Total	C	N	O	S	0	0
			1008	624	201	182	1		

- Molecule 44 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	f	156	Total	C	N	O	S	0	0
			1160	730	213	215	2		

- Molecule 45 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 46 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	63	Total	C	N	O	S	0	0
			516	330	96	87	3		

- Molecule 47 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	g	93	Total	C	N	O	S	0	0
			773	489	136	146	2		

- Molecule 48 is a RNA chain called RNA (5'-R(P*GP*GP*AP*GP*GP*UP*AP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
48	b	9	Total	C	N	O	P	0	0
			199	88	39	63	9		

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	79	Total	C	N	O	S	0	0
			651	413	116	121	1		

- Molecule 51 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 52 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	59	Total	C	N	O	S	0	0
			486	310	88	87	1		

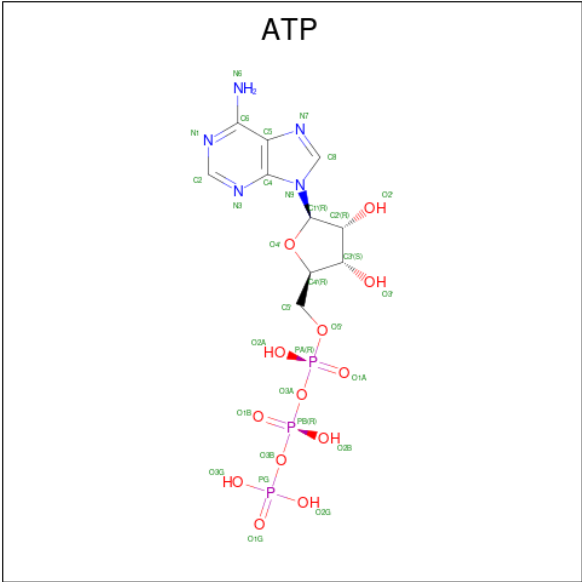
- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	0	2	Total	Mg	0
			2	2	
54	A	115	Total	Mg	0
			115	115	
54	a	19	Total	Mg	0
			19	19	
54	G	1	Total	Mg	0
			1	1	
54	O	1	Total	Mg	0
			1	1	

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
55	0	1	Total	C	N	O	P	0
			31	10	5	13	3	
55	0	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
56	P	1	Total	K	0
			1	1	
56	A	15	Total	K	0
			15	15	
56	a	2	Total	K	0
			2	2	

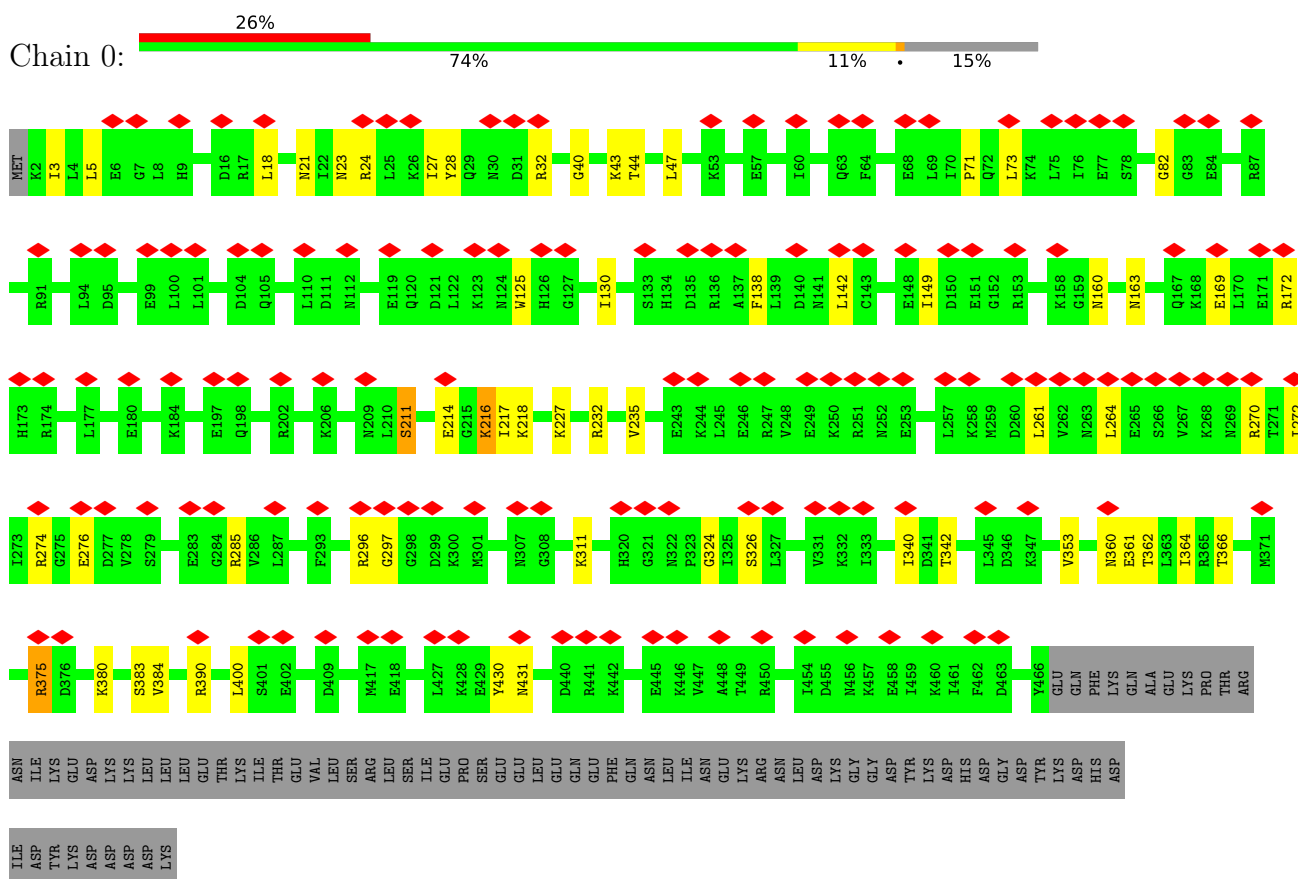
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	6	1	Total	Zn	0
			1	1	
57	o	1	Total	Zn	0
			1	1	
57	9	1	Total	Zn	0
			1	1	
57	5	1	Total	Zn	0
			1	1	

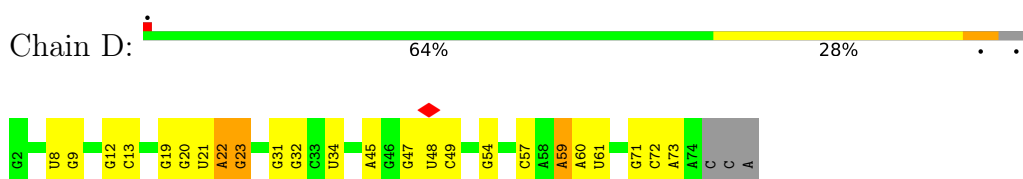
3 Residue-property plots

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: Lincosamide-streptogramin A resistance protein

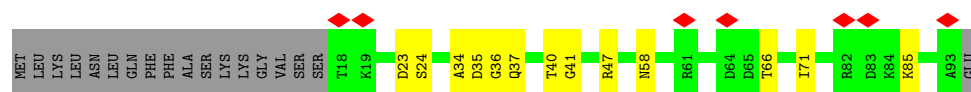


- Molecule 2: P-tRNA fMet

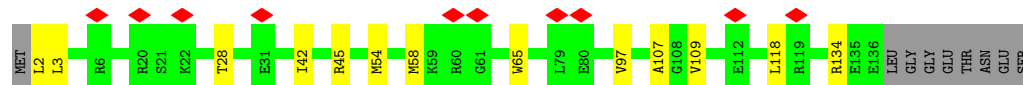
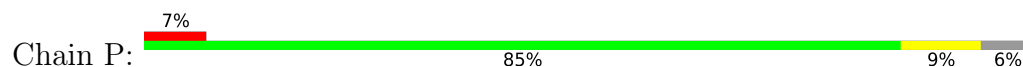


- Molecule 3: 50S ribosomal protein L27

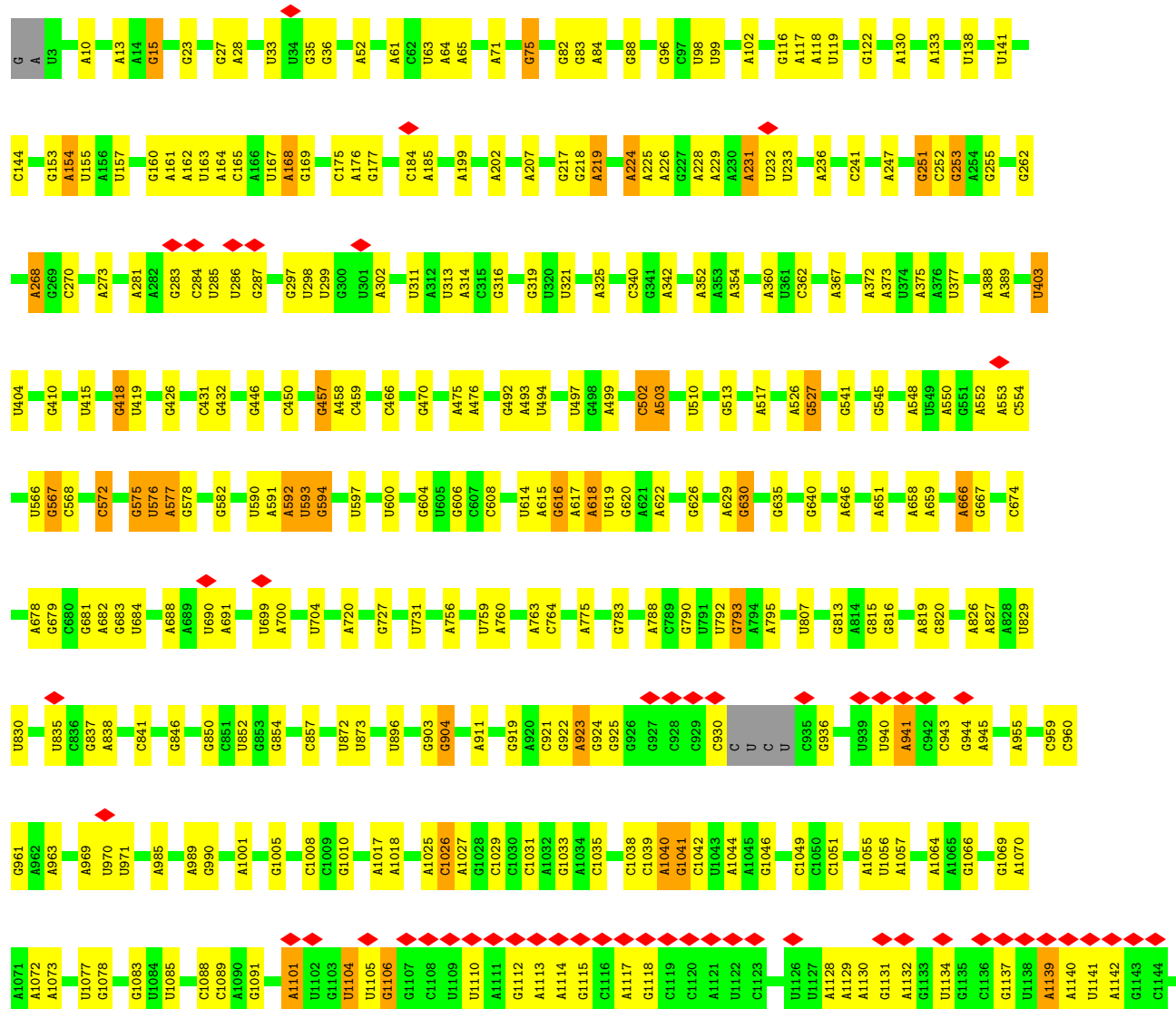




- Molecule 4: 50S ribosomal protein L16



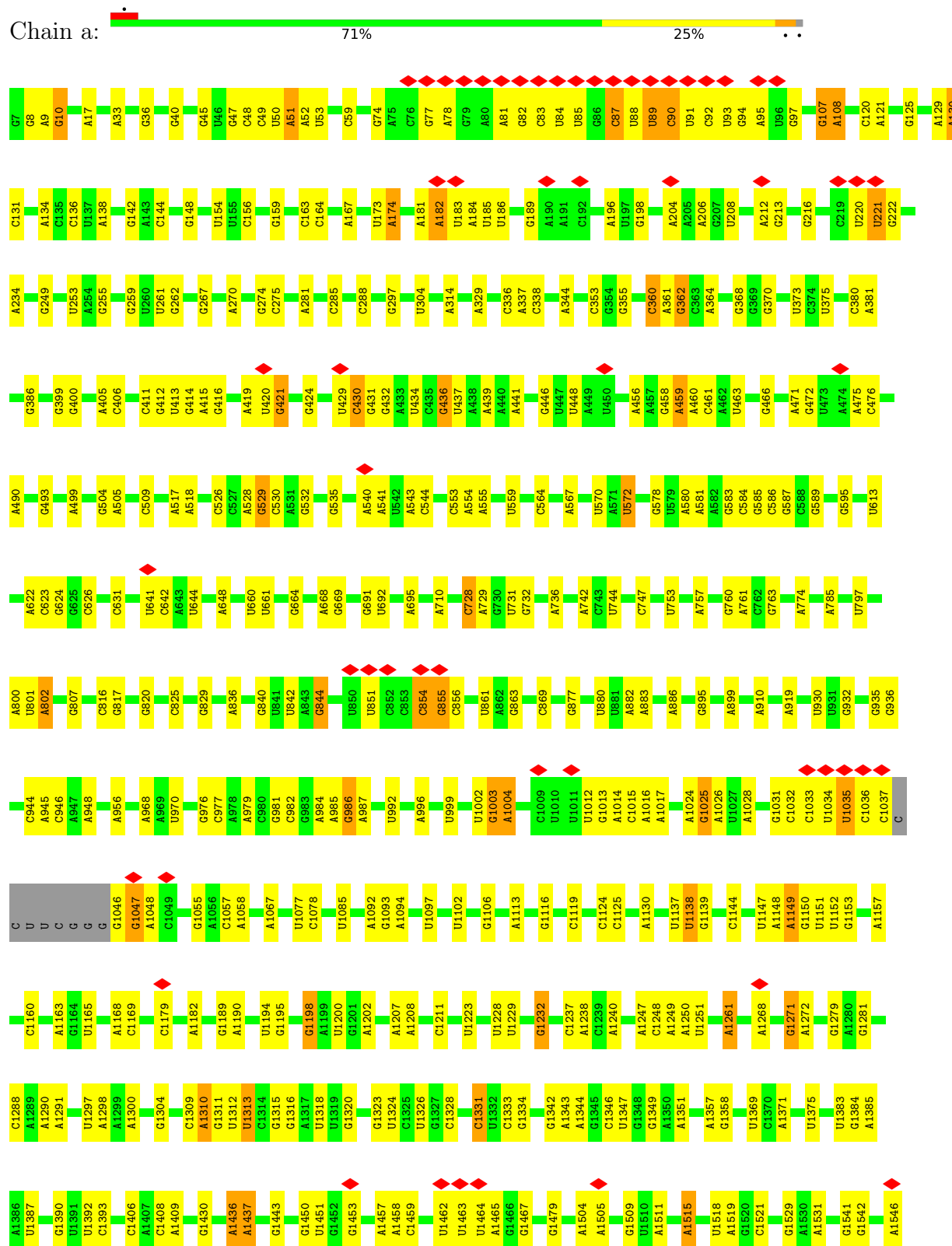
- Molecule 5: 23S rRNA

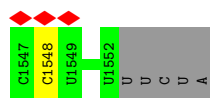


C	A
A2805	A1147
U2806	C1148
U2820	U1149
U2821	C1153
C2822	G1154
C2824	A1155
U2827	G1156
U2831	C1160
C2835	U1163
C2836	G1166
C2838	G1169
A2839	A1170
A2840	A1173
A2841	U1174
G2842	G1175
A2843	U1176
U2844	A1177
C2845	C1178
U2846	C1179
U2847	U1378
U2853	A1379
A2854	G1380
C2856	U1381
A2859	C1382
U2862	C1387
A2869	U1385
A2870	A1386
G2871	G1405
C2872	U1416
U2877	U1431
C2886	A1432
A2887	U1433
U2892	U1434
C2893	A1440
C2894	A1449
A2899	A1450
C2900	C1452
A2903	G1453
U2904	U1454
C2905	U1455
G2906	A1285
A2907	U1286
U2911	U1457
A2912	A1458
G2913	U1292
U2920	U1293
	G1294
	A1303
	G1304
	G1309
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	A1310
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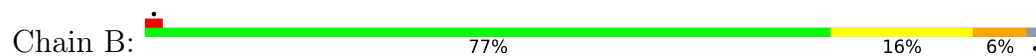
● Molecule 6: 16S rRNA

Chain a:

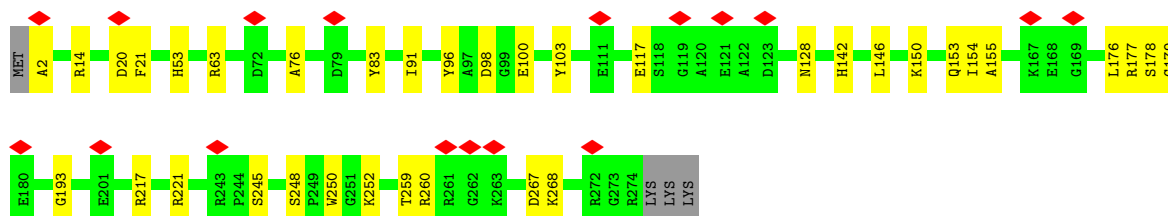
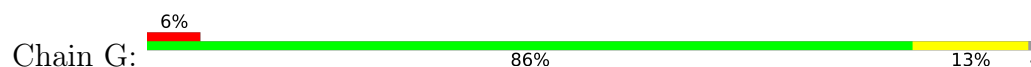




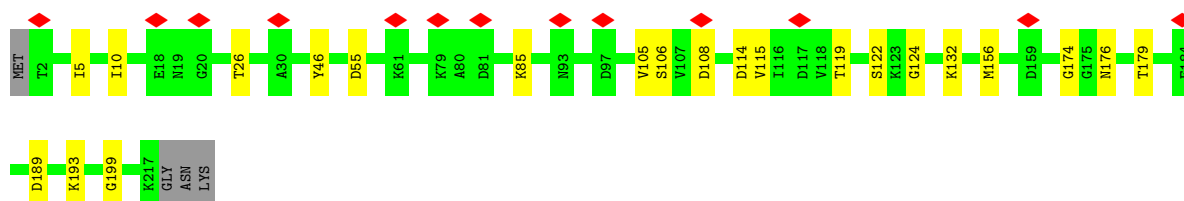
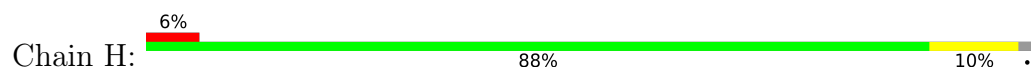
• Molecule 7: 5S rRNA



• Molecule 8: 50S ribosomal protein L2



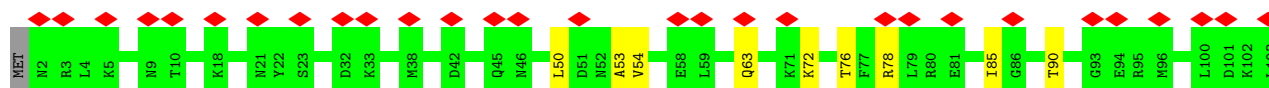
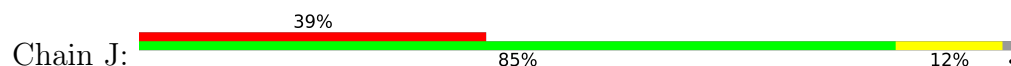
• Molecule 9: 50S ribosomal protein L3

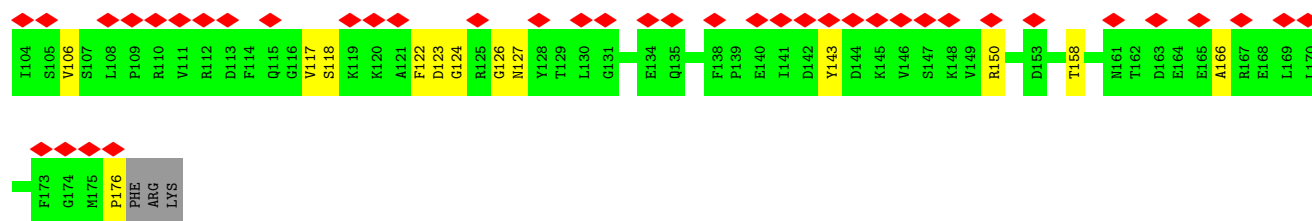


• Molecule 10: 50S ribosomal protein L4

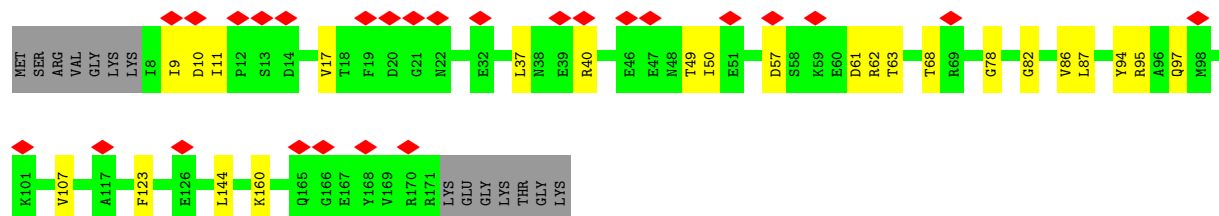
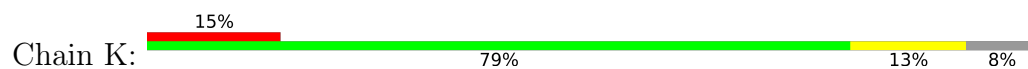


• Molecule 11: 50S ribosomal protein L5

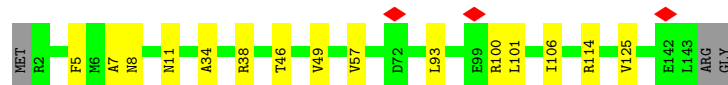
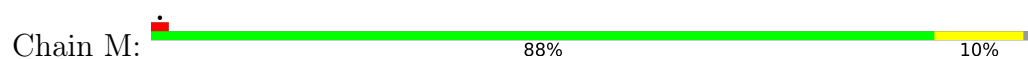




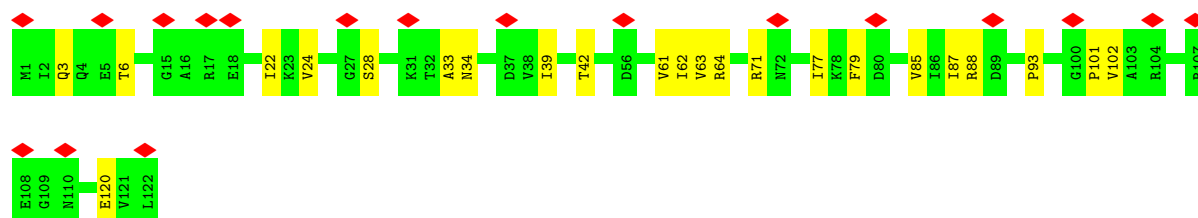
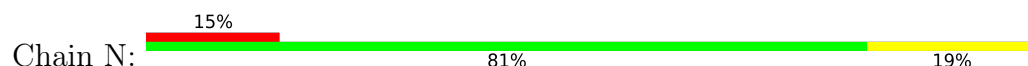
- Molecule 12: 50S ribosomal protein L6



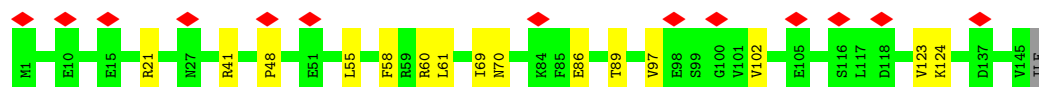
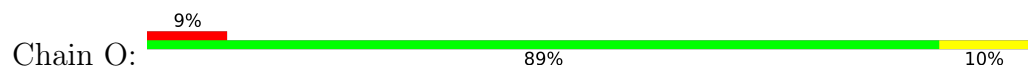
- Molecule 13: 50S ribosomal protein L13



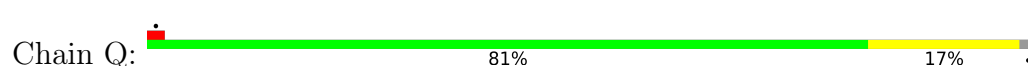
- Molecule 14: 50S ribosomal protein L14



- Molecule 15: 50S ribosomal protein L15

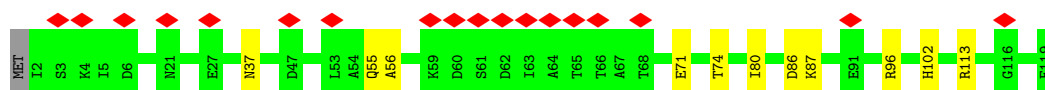
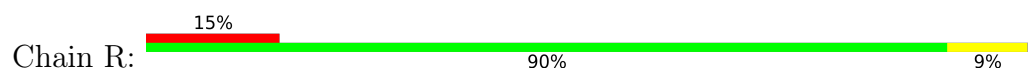


- Molecule 16: 50S ribosomal protein L17

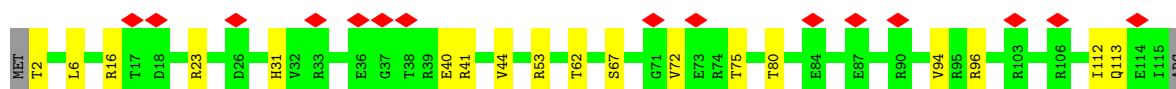
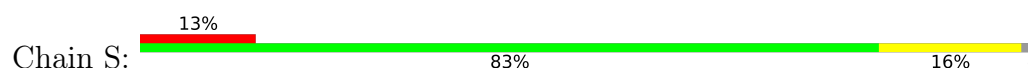




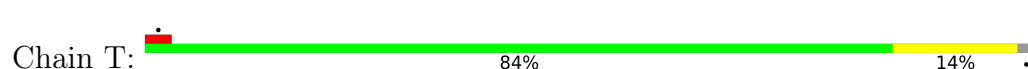
- Molecule 17: 50S ribosomal protein L18



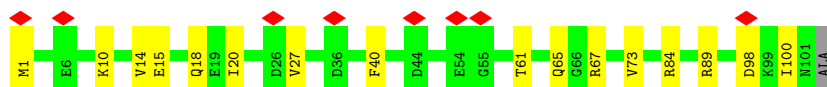
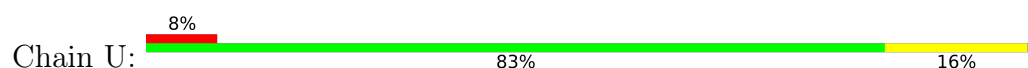
- Molecule 18: 50S ribosomal protein L19



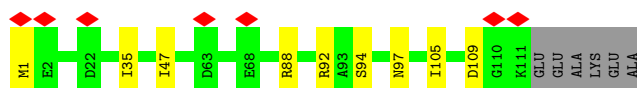
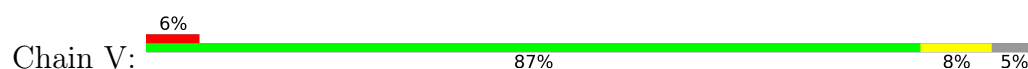
- Molecule 19: 50S ribosomal protein L20



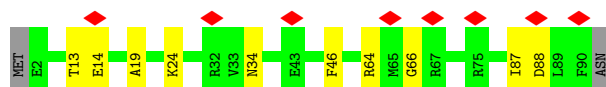
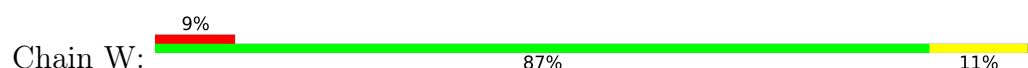
- Molecule 20: 50S ribosomal protein L21



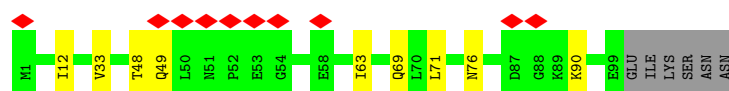
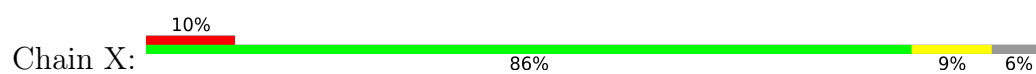
- Molecule 21: 50S ribosomal protein L22



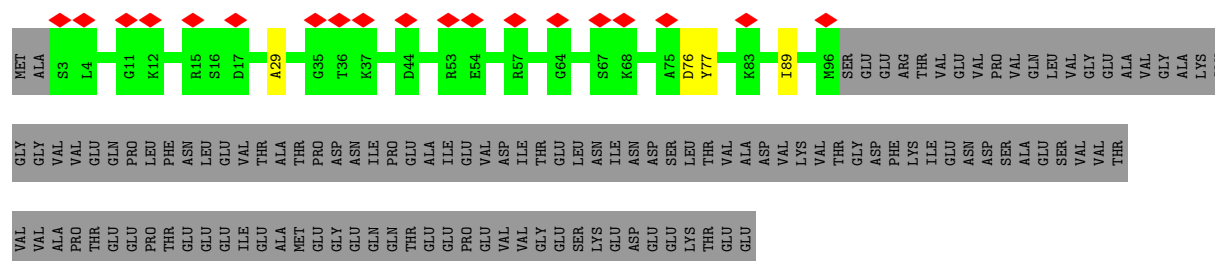
- Molecule 22: 50S ribosomal protein L23



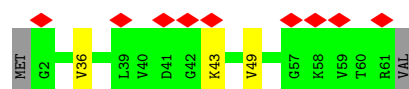
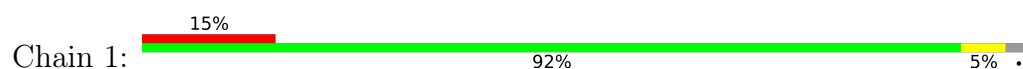
- Molecule 23: 50S ribosomal protein L24



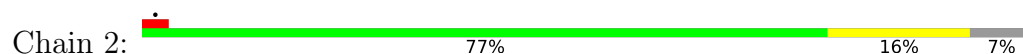
- Molecule 24: 50S ribosomal protein L25



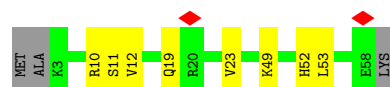
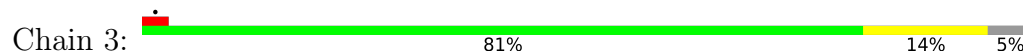
- Molecule 25: 50S ribosomal protein L28



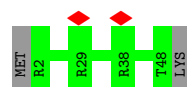
- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L33 2



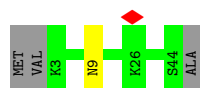
- Molecule 29: 50S ribosomal protein L35

Chain 8:  74% 23% .



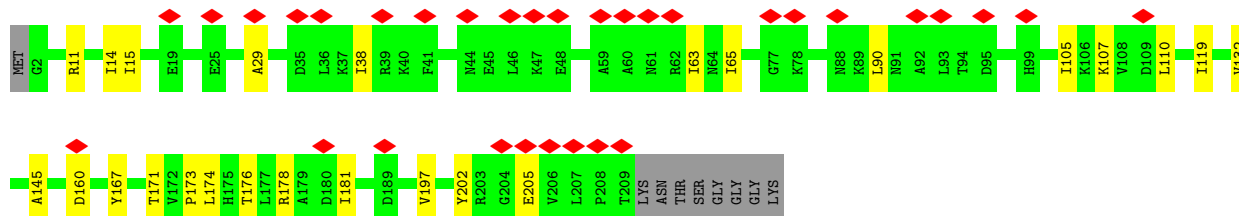
- Molecule 30: 50S ribosomal protein L34

Chain 7:  91% 7% .



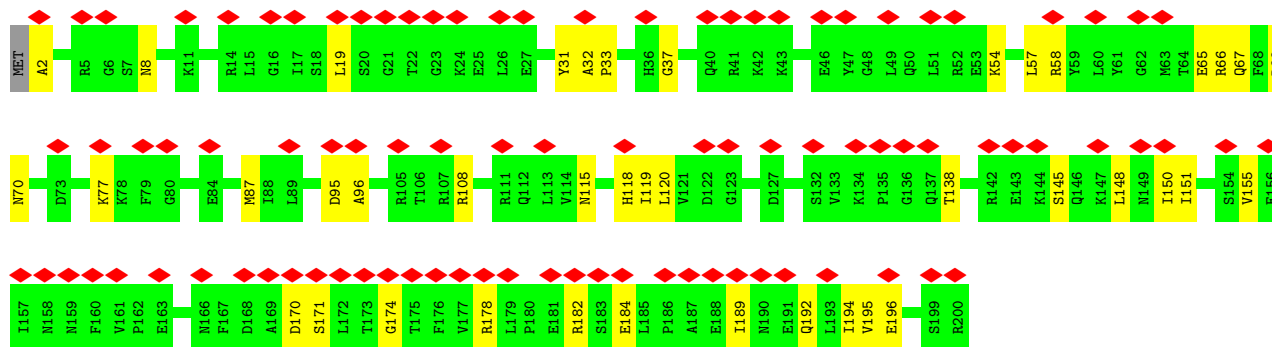
- Molecule 31: 30S ribosomal protein S3

Chain d:  15% 84% 12% .



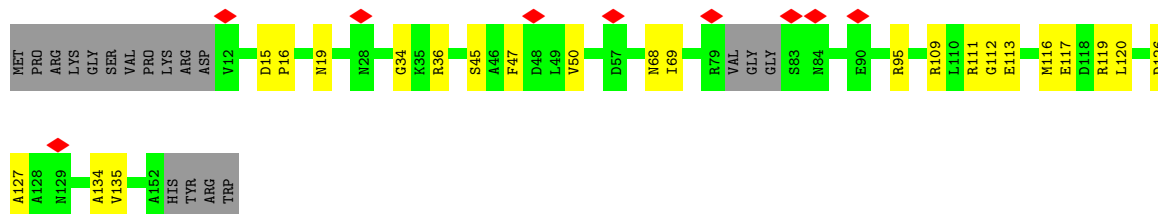
- Molecule 32: 30S ribosomal protein S4

Chain e:  46% 79% 20% .

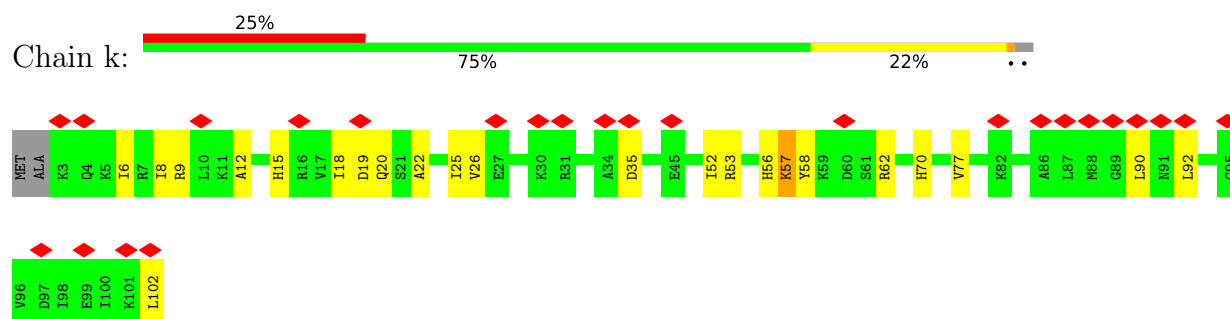


- Molecule 33: 30S ribosomal protein S7

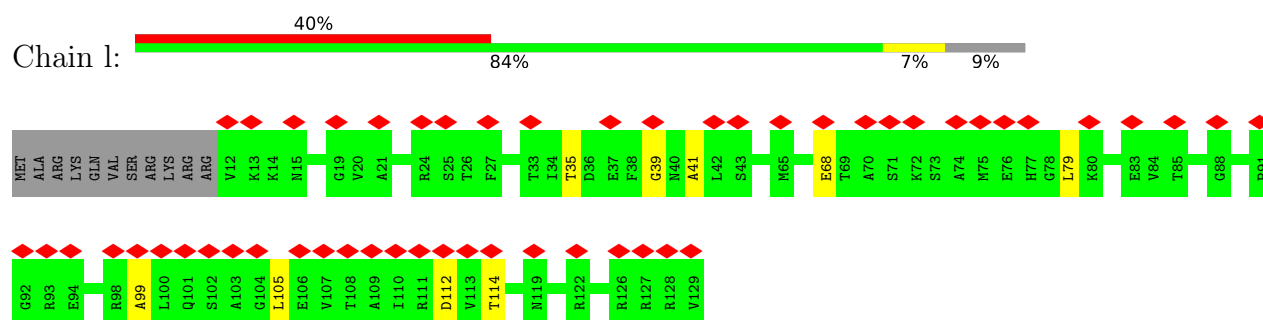
Chain h:  6% 74% 15% 12% .



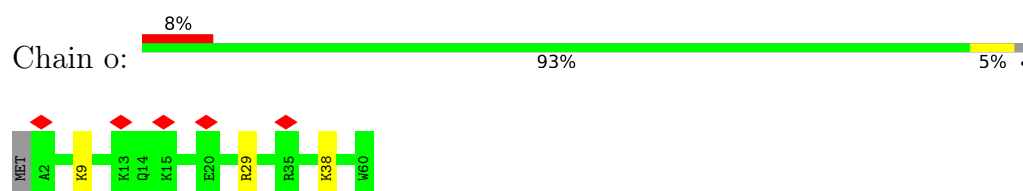
- Molecule 34: 30S ribosomal protein S10



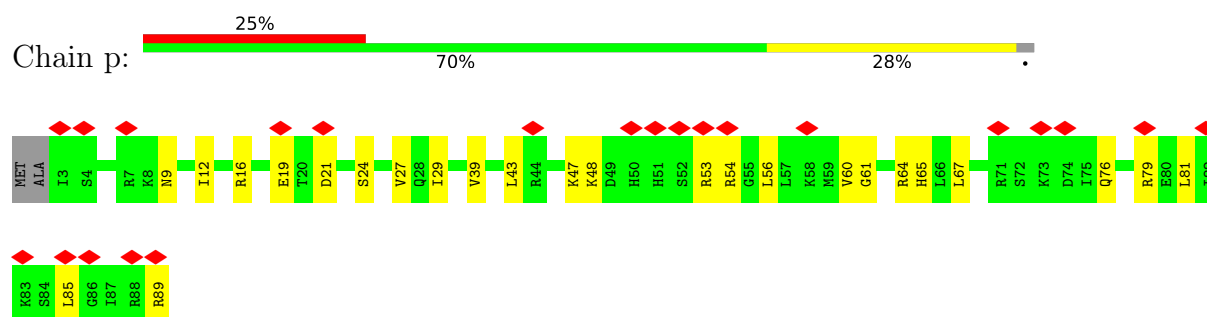
- Molecule 35: 30S ribosomal protein S11



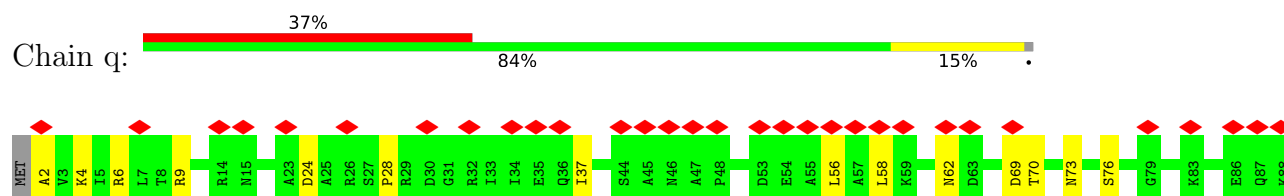
- Molecule 36: 30S ribosomal protein S14 type Z



- Molecule 37: 30S ribosomal protein S15

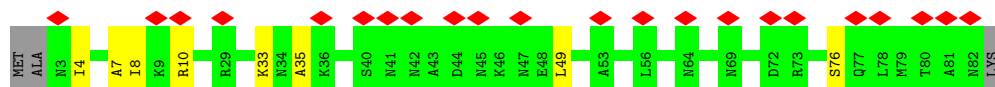
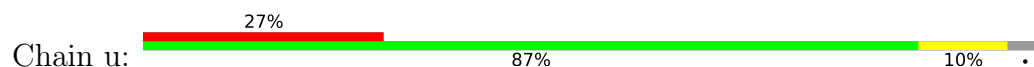


- Molecule 38: 30S ribosomal protein S16

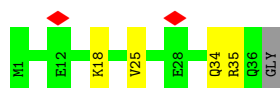
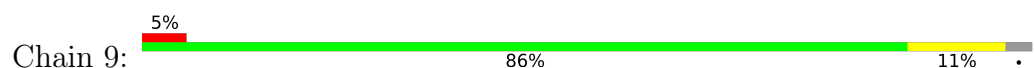




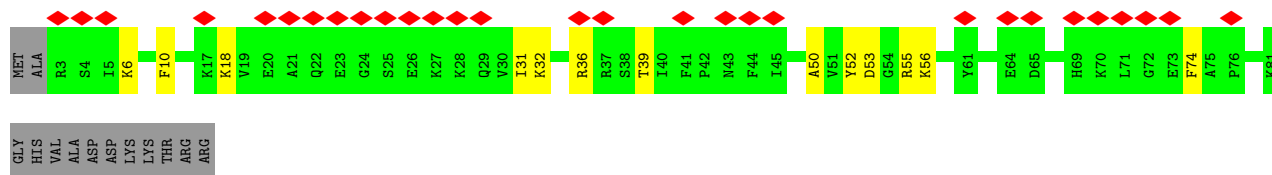
- Molecule 39: 30S ribosomal protein S20



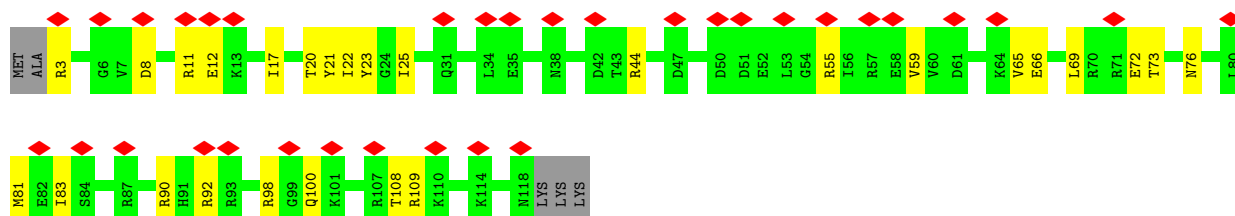
- Molecule 40: 50S ribosomal protein L36



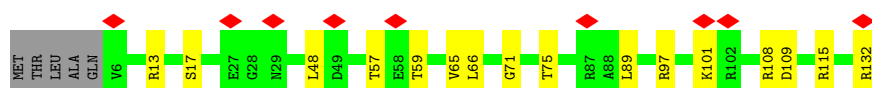
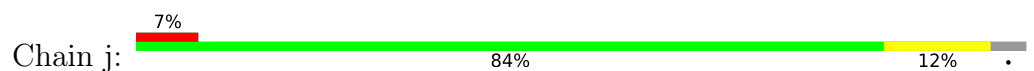
- Molecule 41: 30S ribosomal protein S19



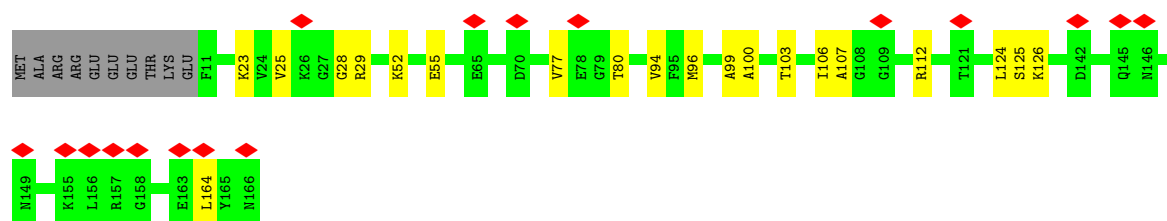
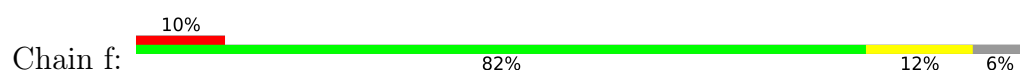
- Molecule 42: 30S ribosomal protein S13



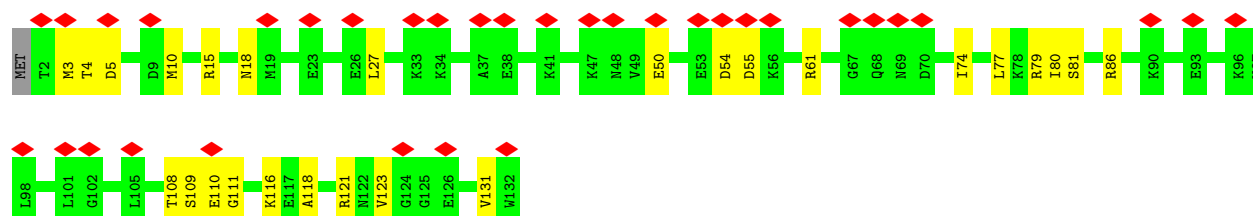
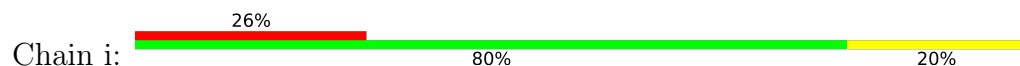
- Molecule 43: 30S ribosomal protein S9



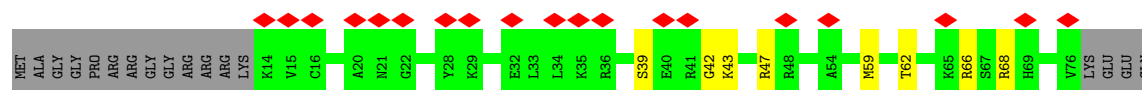
- Molecule 44: 30S ribosomal protein S5



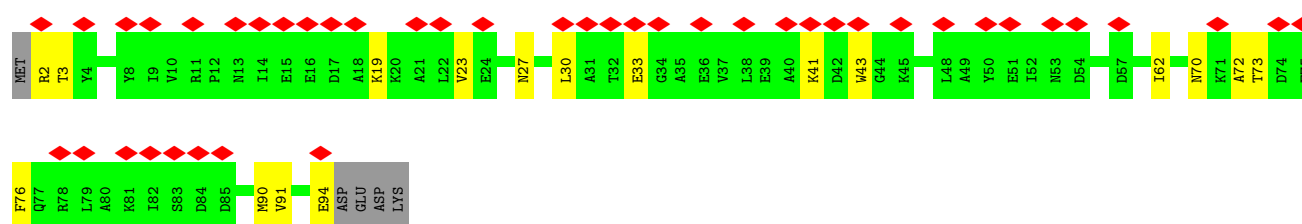
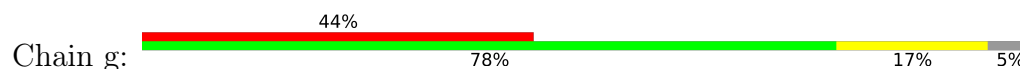
- Molecule 45: 30S ribosomal protein S8



- Molecule 46: 30S ribosomal protein S18



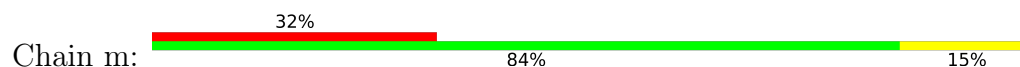
- Molecule 47: 30S ribosomal protein S6



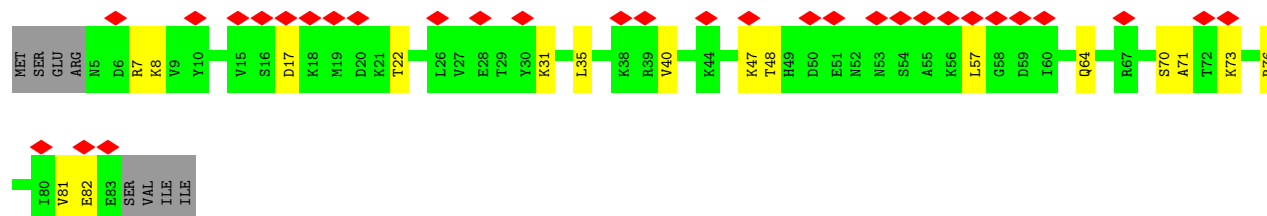
- Molecule 48: RNA (5'-R(P*GP*GP*AP*GP*GP*UP*AP*UP*G)-3')



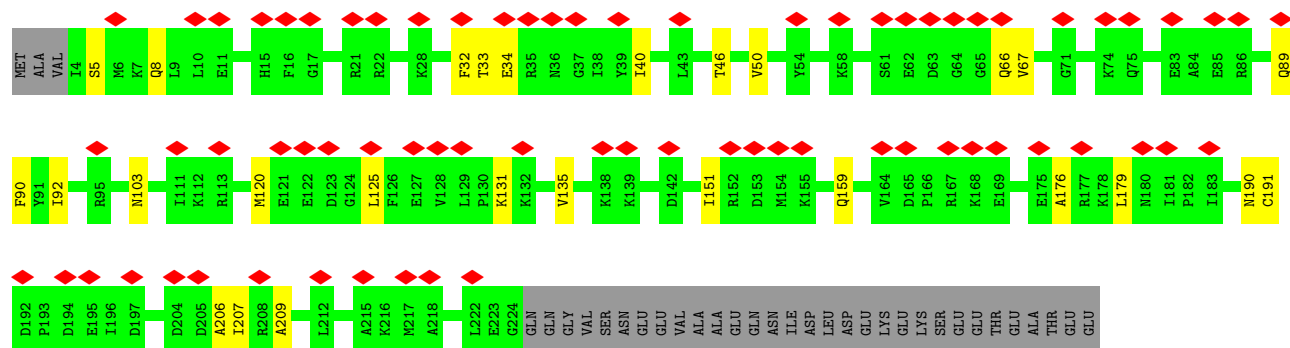
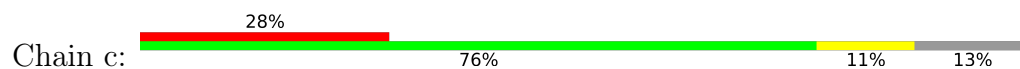
- Molecule 49: 30S ribosomal protein S12



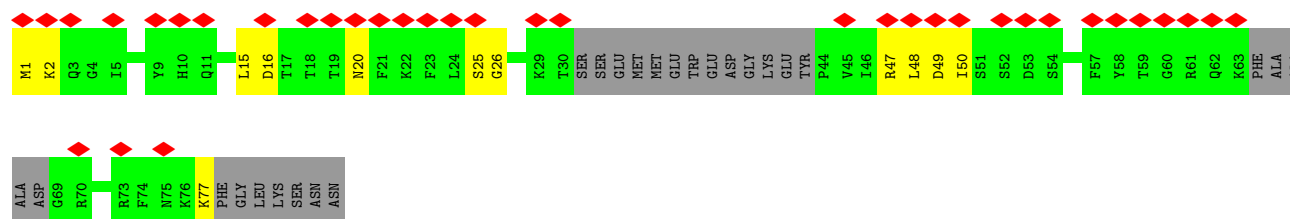
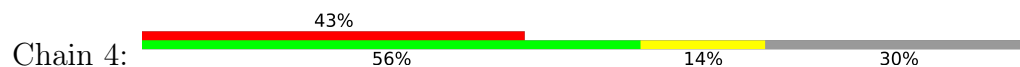
- Molecule 50: 30S ribosomal protein S17



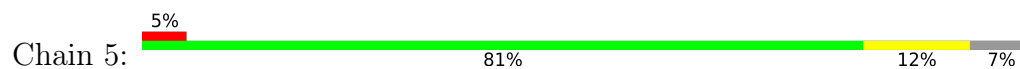
- Molecule 51: 30S ribosomal protein S2

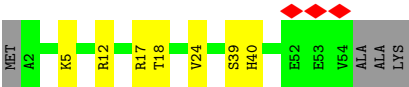


- Molecule 52: 50S ribosomal protein L31 type B



- Molecule 53: 50S ribosomal protein L32





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26.3	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-1900	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	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: K, ZN, ATP, 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	0.55	0/3827	0.72	4/5139 (0.1%)
2	D	0.45	0/1746	0.44	0/2721
3	Z	0.75	0/591	0.64	0/785
4	P	0.74	0/1105	0.61	0/1483
5	A	0.60	0/69977	0.50	0/109141
6	a	0.43	0/36875	0.46	2/57502 (0.0%)
7	B	0.44	0/2692	0.48	0/4193
8	G	0.82	0/2120	0.68	0/2847
9	H	0.77	0/1661	0.61	0/2227
10	I	0.75	0/1587	0.64	0/2143
11	J	0.45	0/1398	0.62	0/1877
12	K	0.44	0/1302	0.52	0/1757
13	M	0.72	0/1149	0.62	0/1549
14	N	0.71	0/927	0.69	0/1243
15	O	0.75	0/1104	0.64	0/1471
16	Q	0.69	0/956	0.66	0/1277
17	R	0.48	0/923	0.61	0/1234
18	S	0.69	0/934	0.68	0/1249
19	T	0.81	0/955	0.66	0/1265
20	U	0.73	0/803	0.60	0/1073
21	V	0.80	0/861	0.68	0/1159
22	W	0.68	0/733	0.62	0/978
23	X	0.54	0/770	0.60	0/1029
24	Y	0.49	0/746	0.61	0/1000
25	1	0.63	0/480	0.73	0/639
26	2	0.56	0/528	0.68	0/703
27	3	0.72	0/438	0.65	0/590
28	6	0.61	0/392	0.60	0/523
29	8	0.82	0/526	0.72	0/690
30	7	0.91	0/364	0.62	0/474
31	d	0.53	0/1661	0.59	0/2233
32	e	0.43	0/1647	0.57	0/2211

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.48	0/1114	0.56	0/1498
34	k	0.51	0/813	0.67	0/1094
35	l	0.40	0/891	0.49	0/1203
36	o	0.58	0/506	0.63	0/671
37	p	0.48	0/742	0.58	0/989
38	q	0.41	0/723	0.59	0/971
39	u	0.42	0/606	0.61	0/810
40	9	0.74	0/295	0.66	0/388
41	t	0.40	0/663	0.52	0/889
42	n	0.44	0/929	0.64	0/1246
43	j	0.53	0/1024	0.66	0/1374
44	f	0.58	0/1174	0.57	0/1583
45	i	0.47	0/1044	0.62	0/1401
46	s	0.48	0/525	0.54	0/704
47	g	0.37	0/784	0.60	0/1052
48	b	0.40	0/222	0.47	0/343
49	m	0.50	0/1075	0.60	0/1439
50	r	0.43	0/659	0.59	0/881
51	c	0.39	0/1808	0.59	0/2426
52	4	0.35	0/496	0.52	0/661
53	5	0.80	0/429	0.70	0/571
All	All	0.56	0/158300	0.52	6/236599 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	71	PRO	N-CA-C	6.89	121.40	111.13
6	a	475	A	C2'-C3'-O3'	6.54	119.31	109.50
1	0	216	LYS	CA-C-N	-5.46	113.36	120.63
1	0	216	LYS	C-N-CA	-5.46	113.36	120.63
6	a	1046	G	C4'-C3'-O3'	5.37	117.45	109.40
1	0	211	SER	O-C-N	5.17	128.52	121.74

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	3770	0	3913	48	0
2	D	1562	0	791	8	0
3	Z	585	0	597	8	0
4	P	1081	0	1143	7	0
5	A	62482	0	31401	235	0
6	a	32937	0	16584	138	0
7	B	2408	0	1218	14	0
8	G	2085	0	2192	27	0
9	H	1637	0	1680	14	0
10	I	1564	0	1611	9	0
11	J	1381	0	1435	17	0
12	K	1284	0	1301	14	0
13	M	1127	0	1117	11	0
14	N	920	0	981	20	0
15	O	1090	0	1131	11	0
16	Q	952	0	999	14	0
17	R	914	0	956	8	0
18	S	922	0	994	13	0
19	T	943	0	1014	12	0
20	U	793	0	831	10	0
21	V	853	0	914	7	0
22	W	725	0	761	7	0
23	X	761	0	823	6	0
24	Y	738	0	787	2	0
25	1	474	0	514	2	0
26	2	527	0	554	7	0
27	3	436	0	473	5	0
28	6	389	0	389	0	0
29	8	521	0	586	13	0
30	7	360	0	406	1	0
31	d	1638	0	1702	17	0
32	e	1617	0	1646	29	0
33	h	1101	0	1133	16	0
34	k	801	0	846	22	0
35	l	876	0	895	6	0
36	o	496	0	518	3	0
37	p	733	0	764	18	0
38	q	712	0	744	8	0
39	u	606	0	650	6	0
40	9	292	0	336	3	0
41	t	646	0	653	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	n	922	0	970	19	0
43	j	1008	0	1031	14	0
44	f	1160	0	1223	14	0
45	i	1032	0	1082	16	0
46	s	516	0	548	5	0
47	g	773	0	772	12	0
48	b	199	0	99	0	0
49	m	1058	0	1130	15	0
50	r	651	0	689	11	0
51	c	1781	0	1844	16	0
52	4	486	0	488	9	0
53	5	422	0	426	7	0
54	0	2	0	0	0	0
54	A	115	0	0	0	0
54	G	1	0	0	0	0
54	O	1	0	0	0	0
54	a	19	0	0	0	0
55	0	62	0	24	11	0
56	A	15	0	0	0	0
56	P	1	0	0	0	0
56	a	2	0	0	0	0
57	5	1	0	0	0	0
57	6	1	0	0	0	0
57	9	1	0	0	0	0
57	o	1	0	0	0	0
All	All	145969	0	98309	783	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 (783) 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)
1:0:311:LYS:NZ	55:0:604:ATP:O1B	1.96	0.97
1:0:380:LYS:NZ	55:0:603:ATP:N3	2.16	0.94
6:a:1200:U:OP1	34:k:53:ARG:NH2	2.11	0.84
4:P:42:ILE:HD12	4:P:97:VAL:HG21	1.59	0.84
5:A:1137:G:H21	5:A:1142:A:H62	1.23	0.84
6:a:81:A:N6	6:a:88:U:O2	2.11	0.83
6:a:220:U:O2'	6:a:221:U:O4'	1.98	0.82
5:A:2477:A:OP1	5:A:2524:A:O2'	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:458:G:OP2	6:a:459:A:O2'	1.98	0.81
1:0:211:SER:HB3	5:A:2582:U:H3	1.46	0.80
5:A:2854:A:N6	5:A:2899:A:O2'	2.15	0.80
5:A:1112:G:N2	5:A:1139:A:O3'	2.15	0.79
47:g:70:ASN:ND2	47:g:73:THR:OG1	2.15	0.79
5:A:2022:U:O2	14:N:3:GLN:NE2	2.15	0.79
5:A:790:G:O2'	5:A:793:G:O2'	2.00	0.79
5:A:2079:G:O2'	9:H:156:MET:O	2.01	0.78
52:4:47:ARG:NH1	52:4:48:LEU:O	2.17	0.77
9:H:55:ASP:OD1	9:H:85:LYS:NZ	2.16	0.77
5:A:253:G:OP2	29:8:13:ARG:NH2	2.17	0.77
44:f:164:LEU:O	45:i:116:LYS:NZ	2.18	0.77
31:d:11:ARG:NH2	31:d:176:THR:O	2.18	0.77
5:A:852:U:OP2	15:O:41:ARG:NH2	2.18	0.77
5:A:1816:A:OP2	8:G:221:ARG:NH2	2.18	0.77
6:a:1229:U:OP1	36:o:9:LYS:NZ	2.18	0.77
5:A:2285:C:O2'	5:A:2454:C:OP2	2.03	0.76
6:a:587:G:O2'	37:p:54:ARG:NH1	2.19	0.76
6:a:399:G:OP1	38:q:9:ARG:NH2	2.17	0.76
12:K:40:ARG:NH1	12:K:61:ASP:OD1	2.18	0.76
7:B:84:U:O2'	7:B:85:U:O2	2.02	0.75
31:d:167:TYR:OH	44:f:55:GLU:OE2	2.05	0.75
5:A:1051:C:OP1	13:M:38:ARG:NH1	2.19	0.75
6:a:1017:A:N6	6:a:1032:C:O2	2.19	0.75
5:A:144:C:OP1	22:W:34:ASN:ND2	2.20	0.74
5:A:678:A:O2'	5:A:2431:C:OP1	2.03	0.74
15:O:55:LEU:O	15:O:60:ARG:NH2	2.19	0.74
5:A:2403:A:N3	17:R:113:ARG:NH2	2.34	0.74
6:a:87:C:O2'	6:a:88:U:O4'	2.05	0.74
5:A:1378:U:OP2	5:A:1431:U:O2'	2.05	0.74
5:A:2329:U:O2'	11:J:123:ASP:O	2.05	0.74
6:a:411:C:OP2	32:e:67:GLN:NE2	2.20	0.74
9:H:26:THR:OG1	9:H:199:GLY:O	2.06	0.74
5:A:2751:U:OP1	9:H:132:LYS:NZ	2.20	0.73
6:a:1190:A:OP2	43:j:97:ARG:NH2	2.21	0.73
5:A:788:A:O2'	5:A:1703:U:OP1	2.07	0.73
1:0:169:GLU:OE2	1:0:172:ARG:NH1	2.21	0.73
5:A:2082:C:OP1	53:5:5:LYS:NZ	2.20	0.73
5:A:704:U:O2'	10:I:101:MET:SD	2.46	0.73
5:A:262:G:HO2'	5:A:666:A:HO2'	1.35	0.73
5:A:2007:G:O2'	5:A:2009:U:OP2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:1313:U:OP2	42:n:21:TYR:OH	2.06	0.73
5:A:84:A:N1	5:A:98:U:O2'	2.19	0.72
5:A:1041:G:OP2	19:T:58:ARG:NH1	2.23	0.72
6:a:1024:A:OP2	41:t:18:LYS:NZ	2.22	0.72
45:i:50:GLU:OE2	45:i:61:ARG:NH2	2.22	0.72
9:H:122:SER:OG	9:H:174:GLY:O	2.07	0.72
6:a:130:A:OP1	50:r:7:ARG:NH2	2.22	0.72
12:K:57:ASP:O	12:K:62:ARG:NH1	2.23	0.72
6:a:182:A:O2'	6:a:184:A:N7	2.23	0.72
6:a:595:G:OP1	45:i:86:ARG:NH2	2.22	0.72
6:a:509:C:OP1	49:m:127:ARG:NH2	2.23	0.72
6:a:986:G:OP2	6:a:1369:U:O2'	2.07	0.72
5:A:1038:C:O2'	5:A:1040:A:OP1	2.07	0.72
5:A:2900:C:O2'	16:Q:96:ARG:NH1	2.22	0.72
6:a:370:G:OP2	49:m:44:ARG:NH1	2.23	0.72
6:a:1093:G:OP2	44:f:52:LYS:NZ	2.23	0.72
20:U:27:VAL:O	20:U:65:GLN:NE2	2.23	0.72
6:a:692:U:O2'	35:l:41:ALA:O	2.05	0.71
9:H:106:SER:OG	9:H:108:ASP:OD1	2.08	0.71
5:A:592:A:O2'	5:A:593:U:O5'	2.07	0.71
6:a:413:U:OP2	32:e:2:ALA:N	2.23	0.71
44:f:107:ALA:O	44:f:112:ARG:NH2	2.24	0.71
1:0:274:ARG:NH1	33:h:112:GLY:O	2.24	0.71
5:A:2231:C:OP2	8:G:150:LYS:NZ	2.20	0.71
5:A:608:C:N3	5:A:619:U:O4	2.24	0.70
6:a:1147:U:N3	6:a:1149:A:OP2	2.24	0.70
29:8:54:ASP:OD1	29:8:57:ARG:NH2	2.24	0.70
5:A:162:A:OP2	5:A:163:U:O2'	2.06	0.70
42:n:12:GLU:O	42:n:44:ARG:NH1	2.23	0.70
5:A:2143:G:O6	5:A:2192:G:O6	2.09	0.70
5:A:2869:G:O6	18:S:23:ARG:NH2	2.25	0.69
10:I:38:ASN:OD1	10:I:41:ARG:NH2	2.25	0.69
5:A:1473:G:OP2	5:A:1606:C:O2'	2.11	0.69
14:N:120:GLU:OE1	18:S:67:SER:OG	2.06	0.69
5:A:2145:U:OP1	5:A:2175:G:O2'	2.10	0.69
6:a:360:C:O2'	6:a:362:G:OP1	2.08	0.69
5:A:720:A:N3	5:A:2470:C:O2'	2.24	0.69
35:l:35:THR:HG22	35:l:41:ALA:HB2	1.74	0.69
1:0:353:VAL:HG11	1:0:364:ILE:HD11	1.75	0.69
5:A:342:A:N3	5:A:362:C:O2'	2.26	0.68
37:p:81:LEU:HD11	37:p:85:LEU:CD1	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2457:A:O2'	5:A:2458:U:O5'	2.11	0.68
20:U:15:GLU:N	20:U:18:GLN:OE1	2.27	0.68
5:A:316:G:O6	5:A:403:U:O2	2.10	0.68
5:A:1361:G:O2'	5:A:1363:U:OP2	2.03	0.68
5:A:1869:G:O2'	8:G:245:SER:OG	2.11	0.68
5:A:2320:C:OP1	17:R:96:ARG:NH1	2.27	0.68
5:A:2863:G:N3	18:S:2:THR:N	2.42	0.68
6:a:1358:G:O2'	6:a:1384:G:O6	2.10	0.68
50:r:64:GLN:OE1	50:r:76:ARG:NH2	2.27	0.68
6:a:1436:A:O2'	6:a:1437:A:O5'	2.09	0.68
4:P:45:ARG:NH2	5:A:2511:G:OP2	2.27	0.68
5:A:759:U:O4	37:p:89:ARG:NH2	2.27	0.68
6:a:381:A:O2'	6:a:459:A:N1	2.27	0.68
6:a:1067:A:O2'	31:d:160:ASP:O	2.11	0.68
10:I:142:VAL:O	10:I:145:THR:OG1	2.09	0.68
11:J:126:GLY:O	11:J:158:THR:OG1	2.11	0.67
29:8:17:THR:OG1	29:8:18:ALA:O	2.06	0.67
45:i:18:ASN:ND2	45:i:74:ILE:O	2.27	0.67
5:A:1711:G:O2'	5:A:2018:U:O4	2.13	0.67
5:A:2666:A:O2'	13:M:100:ARG:NH1	2.28	0.67
2:D:59:A:O2'	2:D:61:U:OP2	2.12	0.67
5:A:575:G:O2'	5:A:577:A:N7	2.26	0.67
6:a:36:G:O2'	49:m:128:SER:O	2.07	0.67
1:0:5:LEU:HD23	1:0:27:ILE:HD11	1.77	0.67
1:0:383:SER:O	1:0:390:ARG:NH2	2.27	0.67
6:a:1025:G:O2'	6:a:1229:U:O2'	2.13	0.67
16:Q:109:ARG:O	16:Q:113:GLY:HA2	1.94	0.67
6:a:415:A:OP1	32:e:108:ARG:NH2	2.27	0.67
6:a:1331:C:N3	41:t:36:ARG:NH1	2.42	0.67
5:A:1472:C:O2'	5:A:1616:A:OP2	2.08	0.66
7:B:81:A:H61	7:B:90:U:H3	1.43	0.66
7:B:111:C:O2'	17:R:55:GLN:OE1	2.04	0.66
37:p:81:LEU:HD11	37:p:85:LEU:HD11	1.77	0.66
5:A:896:U:OP1	27:3:49:LYS:NZ	2.29	0.66
14:N:22:ILE:HD11	14:N:42:THR:HG23	1.77	0.66
5:A:635:G:O2'	29:8:64:TYR:OH	2.13	0.66
5:A:815:G:OP1	30:7:9:ASN:ND2	2.28	0.66
5:A:1712:A:O2'	5:A:1718:G:N7	2.26	0.66
5:A:1169:G:OP2	5:A:1170:A:O2'	2.07	0.66
6:a:1189:G:OP2	43:j:101:LYS:NZ	2.25	0.66
8:G:63:ARG:NH1	8:G:83:TYR:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:296:ARG:NH1	33:h:111:ARG:O	2.29	0.66
5:A:593:U:O2'	5:A:594:G:OP1	2.12	0.66
32:e:57:LEU:HD21	32:e:87:MET:HE1	1.77	0.66
41:t:10:PHE:O	41:t:39:THR:OG1	2.10	0.65
8:G:142:HIS:ND1	8:G:193:GLY:O	2.30	0.65
42:n:81:MET:O	42:n:92:ARG:NH2	2.29	0.65
5:A:2160:G:O2'	5:A:2161:A:OP2	2.14	0.65
6:a:107:G:N2	6:a:108:A:N1	2.45	0.65
6:a:644:U:OP1	50:r:8:LYS:NZ	2.30	0.65
1:0:211:SER:HB3	5:A:2582:U:N3	2.12	0.65
34:k:6:ILE:HG23	34:k:102:LEU:HD21	1.77	0.65
52:4:16:ASP:O	52:4:20:ASN:N	2.29	0.65
6:a:1443:G:HO2'	6:a:1479:G:H1	1.41	0.65
38:q:2:ALA:N	38:q:24:ASP:OD1	2.30	0.65
3:Z:85:LYS:NZ	5:A:903:G:OP2	2.30	0.65
44:f:100:ALA:O	44:f:103:THR:OG1	2.13	0.65
5:A:2138:U:OP2	5:A:2172:C:N4	2.29	0.64
5:A:2663:U:O2'	9:H:46:TYR:OH	2.14	0.64
42:n:22:ILE:HG21	42:n:25:ILE:HD12	1.79	0.64
21:V:47:ILE:HG23	21:V:105:ILE:HD11	1.78	0.64
1:0:82:GLY:O	55:0:604:ATP:O3G	2.15	0.64
1:0:3:ILE:HD11	5:A:1886:A:N3	2.13	0.64
5:A:1008:C:O2'	5:A:2300:A:N3	2.29	0.64
5:A:1137:G:N2	5:A:1142:A:H62	1.93	0.64
16:Q:101:THR:OG1	16:Q:120:GLU:O	2.10	0.64
5:A:1078:G:OP2	40:9:18:LYS:NZ	2.30	0.64
5:A:568:C:O2	5:A:597:U:O2'	2.16	0.64
5:A:600:U:OP1	13:M:114:ARG:NH1	2.31	0.64
39:u:4:ILE:HD12	39:u:8:ILE:HG21	1.80	0.64
5:A:352:A:N3	5:A:372:A:O2'	2.29	0.64
5:A:2686:G:N2	5:A:2689:A:OP2	2.31	0.64
42:n:17:ILE:O	42:n:20:THR:OG1	2.14	0.64
45:i:108:THR:OG1	45:i:111:GLY:O	2.16	0.64
5:A:1658:A:N6	21:V:92:ARG:O	2.31	0.63
5:A:2836:C:O2	5:A:2903:A:O2'	2.16	0.63
5:A:925:G:O6	5:A:941:A:N1	2.31	0.63
34:k:8:ILE:HD12	34:k:25:ILE:HD12	1.78	0.63
5:A:2769:G:OP1	40:9:35:ARG:NH1	2.32	0.63
15:O:61:LEU:O	29:8:13:ARG:NH1	2.31	0.63
6:a:125:G:OP1	6:a:613:U:O2'	2.15	0.63
5:A:904:G:O2'	5:A:961:G:O6	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1725:G:O2'	5:A:1789:A:O2'	2.08	0.63
6:a:728:C:OP2	6:a:729:A:O2'	2.06	0.63
5:A:224:A:N1	5:A:268:A:O2'	2.31	0.63
6:a:1310:A:O2'	6:a:1312:U:O4'	2.15	0.63
17:R:71:GLU:O	17:R:74:THR:OG1	2.14	0.63
5:A:1104:U:N3	5:A:1106:G:O4'	2.32	0.63
6:a:541:A:O2'	6:a:543:A:OP2	2.13	0.62
7:B:40:C:N3	11:J:90:THR:OG1	2.31	0.62
33:h:15:ASP:OD1	33:h:19:ASN:N	2.32	0.62
46:s:59:MET:O	46:s:62:THR:OG1	2.17	0.62
5:A:2842:G:O2'	5:A:2844:U:OP2	2.08	0.62
11:J:106:VAL:HG13	52:4:48:LEU:HD22	1.80	0.62
49:m:61:ALA:HB3	49:m:63:ARG:HH22	1.65	0.62
1:0:375:ARG:HB3	2:D:57:C:N4	2.15	0.62
1:0:232:ARG:O	1:0:235:VAL:HG22	2.00	0.62
5:A:1173:A:O2'	5:A:2542:C:O2	2.15	0.62
2:D:22:A:O2'	2:D:23:G:O5'	2.16	0.62
49:m:81:PRO:O	49:m:112:ARG:NH2	2.32	0.62
5:A:1710:G:O2'	14:N:6:THR:HG22	2.00	0.62
34:k:57:LYS:NZ	34:k:58:TYR:CZ	2.66	0.62
6:a:1408:C:OP2	44:f:29:ARG:NH2	2.33	0.61
5:A:2251:G:OP1	8:G:268:LYS:NZ	2.25	0.61
6:a:386:G:OP2	38:q:4:LYS:NZ	2.33	0.61
6:a:1138:U:HO2'	6:a:1291:A:HO2'	1.44	0.61
52:4:15:LEU:O	52:4:48:LEU:N	2.34	0.61
5:A:2060:A:O2'	5:A:2062:G:OP2	2.13	0.61
50:r:70:SER:OG	50:r:71:ALA:O	2.17	0.61
37:p:21:ASP:OD2	37:p:24:SER:OG	2.14	0.61
42:n:72:GLU:OE2	42:n:76:ASN:ND2	2.33	0.61
5:A:1824:C:O2'	8:G:259:THR:OG1	2.19	0.61
5:A:2074:C:O2'	5:A:2843:A:N1	2.32	0.61
5:A:760:A:OP2	37:p:64:ARG:NH2	2.33	0.61
5:A:2649:U:O2'	5:A:2845:G:N7	2.34	0.61
8:G:248:SER:OG	8:G:250:TRP:O	2.18	0.61
21:V:1:MET:N	21:V:109:ASP:OD1	2.34	0.61
5:A:75:G:OP1	26:2:44:ARG:NH1	2.34	0.60
5:A:168:A:O5'	25:1:43:LYS:NZ	2.34	0.60
6:a:9:A:N6	32:e:196:GLU:O	2.34	0.60
5:A:241:C:O2'	5:A:651:A:N3	2.35	0.60
5:A:2326:G:OP1	11:J:72:LYS:NZ	2.23	0.60
5:A:2332:U:N3	11:J:150:ARG:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2710:C:OP1	18:S:53:ARG:NH1	2.33	0.60
22:W:19:ALA:HB1	22:W:24:LYS:HB2	1.82	0.60
6:a:816:C:OP2	37:p:48:LYS:NZ	2.30	0.60
33:h:68:ASN:ND2	33:h:127:ALA:O	2.33	0.60
51:c:120:MET:O	51:c:125:LEU:N	2.34	0.60
6:a:800:A:O2'	6:a:802:A:N7	2.27	0.60
38:q:58:LEU:O	38:q:62:ASN:ND2	2.35	0.60
2:D:34:U:OP2	43:j:132:ARG:NH1	2.34	0.60
43:j:108:ARG:NH2	43:j:109:ASP:O	2.35	0.60
1:0:340:ILE:HG22	1:0:342:THR:H	1.67	0.59
14:N:24:VAL:HG11	14:N:33:ALA:HB2	1.83	0.59
18:S:62:THR:HB	18:S:75:THR:HG22	1.84	0.59
5:A:1781:C:N3	5:A:2743:U:O2'	2.31	0.59
6:a:1003:G:O2'	6:a:1004:A:N7	2.35	0.59
5:A:138:U:N3	5:A:141:U:OP2	2.35	0.59
6:a:434:U:OP1	32:e:31:TYR:OH	2.21	0.59
11:J:143:TYR:OH	42:n:3:ARG:NH2	2.36	0.59
1:0:274:ARG:O	1:0:326:SER:N	2.35	0.59
20:U:67:ARG:O	20:U:89:ARG:NH2	2.35	0.59
42:n:23:TYR:CE2	42:n:69:LEU:HD22	2.38	0.59
1:0:270:ARG:NH1	6:a:1309:C:O2	2.35	0.59
5:A:969:A:O2'	5:A:971:U:OP2	2.21	0.59
16:Q:90:ALA:O	16:Q:94:THR:HG23	2.03	0.58
14:N:24:VAL:CG1	14:N:33:ALA:HB2	2.33	0.58
6:a:554:A:OP2	32:e:58:ARG:NH2	2.36	0.58
6:a:1318:U:OP1	42:n:100:GLN:NE2	2.36	0.58
37:p:29:ILE:HD13	37:p:67:LEU:HD13	1.85	0.58
16:Q:50:LEU:HD23	16:Q:62:ALA:HB2	1.86	0.58
51:c:176:ALA:O	51:c:179:LEU:N	2.37	0.58
3:Z:35:ASP:OD1	3:Z:36:GLY:N	2.36	0.58
1:0:43:LYS:HG2	1:0:149:ILE:HD12	1.86	0.58
32:e:182:ARG:NH2	32:e:189:ILE:O	2.36	0.58
5:A:1543:G:N2	8:G:98:ASP:O	2.37	0.57
23:X:12:ILE:HD11	23:X:69:GLN:HB2	1.84	0.57
26:2:10:THR:OG1	26:2:13:GLU:OE1	2.08	0.57
34:k:56:HIS:HD2	34:k:57:LYS:HG3	1.69	0.57
44:f:99:ALA:HB2	44:f:124:LEU:HD13	1.86	0.57
5:A:2432:G:O2'	5:A:2433:C:OP2	2.12	0.57
6:a:1085:U:O2	51:c:103:ASN:ND2	2.37	0.57
5:A:688:A:N1	5:A:2396:A:O2'	2.38	0.57
5:A:1462:G:O2'	5:A:1626:A:N6	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:47:G:O2'	6:a:373:U:O2	2.23	0.57
49:m:24:LEU:O	49:m:40:SER:OG	2.10	0.57
5:A:2820:U:O2'	5:A:2821:U:O2	2.18	0.57
14:N:39:ILE:HD11	14:N:62:ILE:HD11	1.87	0.57
33:h:111:ARG:NH1	33:h:126:ASP:OD2	2.37	0.57
51:c:5:SER:N	51:c:8:GLN:OE1	2.38	0.57
5:A:1696:C:OP1	16:Q:4:ARG:NH1	2.36	0.57
6:a:77:G:O2'	6:a:78:A:O4'	2.19	0.56
42:n:65:VAL:HG12	42:n:66:GLU:H	1.70	0.56
46:s:42:GLY:O	46:s:68:ARG:NH2	2.38	0.56
50:r:22:THR:OG1	50:r:48:THR:O	2.12	0.56
51:c:66:GLN:N	51:c:159:GLN:OE1	2.37	0.56
5:A:226:A:O2'	5:A:466:C:O2	2.22	0.56
6:a:996:A:N3	41:t:52:TYR:OH	2.33	0.56
20:U:1:MET:HE1	20:U:100:ILE:HB	1.88	0.56
1:0:375:ARG:HB3	2:D:57:C:H41	1.70	0.56
5:A:1540:U:O2'	5:A:1625:U:OP1	2.21	0.56
5:A:340:C:OP1	23:X:90:LYS:NZ	2.30	0.56
29:8:26:ARG:HE	29:8:44:LEU:HD23	1.70	0.56
5:A:82:G:N2	5:A:102:A:OP2	2.35	0.56
32:e:118:HIS:NE2	32:e:145:SER:O	2.38	0.56
49:m:91:SER:OG	49:m:116:ASP:OD2	2.20	0.56
32:e:148:LEU:HB2	32:e:151:ILE:HD13	1.88	0.55
5:A:1042:C:OP2	19:T:58:ARG:NH2	2.38	0.55
5:A:630:G:OP2	15:O:21:ARG:NH1	2.36	0.55
6:a:935:G:N2	6:a:1515:A:OP1	2.40	0.55
31:d:178:ARG:NE	31:d:205:GLU:OE2	2.37	0.55
2:D:31:G:OP1	6:a:1240:A:O2'	2.24	0.55
6:a:984:A:OP1	36:o:29:ARG:NH2	2.39	0.55
22:W:64:ARG:NH1	22:W:66:GLY:O	2.38	0.55
16:Q:26:ILE:HG23	16:Q:71:ILE:HD13	1.87	0.55
35:l:112:ASP:OD1	35:l:114:THR:OG1	2.14	0.55
5:A:2277:G:O2'	5:A:2523:C:OP1	2.19	0.55
6:a:530:C:H41	49:m:63:ARG:HH11	1.55	0.55
7:B:32:U:O2'	7:B:42:G:N7	2.39	0.55
5:A:545:G:N1	5:A:548:A:OP2	2.40	0.55
5:A:2048:G:OP2	53:5:12:ARG:NE	2.40	0.55
5:A:2593:A:N1	14:N:28:SER:OG	2.40	0.55
6:a:774:A:OP2	6:a:820:G:N2	2.40	0.54
5:A:251:G:O2'	5:A:2459:A:OP1	2.18	0.54
6:a:430:C:O4'	6:a:431:G:N2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:p:47:LYS:O	37:p:53:ARG:NH1	2.38	0.54
1:0:218:LYS:NZ	5:A:2520:U:OP2	2.33	0.54
5:A:838:A:OP2	5:A:2098:A:O2'	2.24	0.54
5:A:1072:A:H2'	5:A:1073:A:C8	2.42	0.54
19:T:50:ARG:O	19:T:54:LYS:NZ	2.41	0.54
5:A:527:G:O2'	5:A:552:A:N6	2.41	0.54
6:a:529:G:O2'	6:a:544:C:O2'	2.26	0.54
34:k:6:ILE:HG23	34:k:102:LEU:CD2	2.36	0.54
37:p:61:GLY:O	37:p:65:HIS:ND1	2.41	0.54
32:e:178:ARG:NH1	32:e:184:GLU:OE2	2.41	0.54
34:k:35:ASP:O	34:k:77:VAL:N	2.40	0.54
5:A:2189:G:O2'	5:A:2190:C:O4'	2.20	0.54
5:A:65:A:O2'	5:A:502:C:N3	2.38	0.54
5:A:1432:A:O2'	5:A:1434:U:OP2	2.25	0.54
43:j:17:SER:OG	43:j:71:GLY:O	2.21	0.54
5:A:1010:G:O4'	5:A:2294:A:N6	2.40	0.54
7:B:35:C:O2	17:R:102:HIS:NE2	2.39	0.54
12:K:9:ILE:O	12:K:49:THR:OG1	2.20	0.54
18:S:40:GLU:O	18:S:41:ARG:NE	2.39	0.54
1:0:362:THR:O	1:0:366:THR:OG1	2.13	0.53
5:A:2347:A:O2'	5:A:2348:G:OP2	2.23	0.53
6:a:553:C:OP1	32:e:54:LYS:NZ	2.40	0.53
5:A:33:U:O4	5:A:492:G:O2'	2.22	0.53
6:a:17:A:N3	6:a:1092:A:O2'	2.39	0.53
6:a:1271:G:O2'	6:a:1272:A:OP2	2.23	0.53
5:A:27:G:O2'	5:A:28:A:OP2	2.21	0.53
10:I:6:VAL:C	10:I:7:LEU:HD12	2.33	0.53
26:2:2:LYS:NZ	26:2:5:GLU:OE1	2.42	0.53
5:A:1938:U:O2'	5:A:1939:A:OP1	2.23	0.53
5:A:2590:U:O2'	5:A:2592:A:N7	2.39	0.53
8:G:117:GLU:N	8:G:128:ASN:OD1	2.40	0.53
29:8:9:GLY:O	29:8:13:ARG:NE	2.41	0.53
5:A:10:A:N6	5:A:2655:U:OP1	2.41	0.53
5:A:1452:C:N4	5:A:1632:A:N6	2.57	0.53
20:U:61:THR:OG1	20:U:98:ASP:OD2	2.26	0.53
26:2:10:THR:O	26:2:11:THR:OG1	2.17	0.53
5:A:262:G:O2'	5:A:666:A:O2'	2.09	0.53
6:a:1163:A:OP1	34:k:70:HIS:ND1	2.41	0.53
11:J:53:ALA:HB2	11:J:150:ARG:NE	2.24	0.53
16:Q:26:ILE:CG2	16:Q:71:ILE:HD13	2.39	0.53
31:d:173:PRO:O	31:d:176:THR:OG1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:15:HIS:HA	34:k:18:ILE:HG22	1.91	0.53
6:a:1094:A:OP1	44:f:23:LYS:NZ	2.41	0.53
6:a:1323:G:OP2	52:4:77:LYS:NZ	2.41	0.53
1:0:32:ARG:NH1	1:0:125:TRP:O	2.41	0.52
5:A:1534:G:O2'	8:G:100:GLU:OE2	2.13	0.52
6:a:1288:C:O2'	6:a:1290:A:N7	2.41	0.52
13:M:93:LEU:HD23	13:M:101:LEU:HD13	1.91	0.52
38:q:37:ILE:HG22	38:q:56:LEU:HG	1.90	0.52
1:0:384:VAL:CG1	55:0:603:ATP:C5	2.91	0.52
5:A:2238:U:O2'	5:A:2239:A:O4'	2.27	0.52
14:N:64:ARG:NH2	14:N:101:PRO:O	2.41	0.52
31:d:110:LEU:HD11	31:d:145:ALA:HB2	1.91	0.52
35:l:79:LEU:HD23	35:l:105:LEU:HD13	1.91	0.52
39:u:35:ALA:HA	39:u:49:LEU:HD23	1.91	0.52
23:X:33:VAL:N	23:X:63:ILE:O	2.41	0.52
45:i:77:LEU:HD23	45:i:131:VAL:HG13	1.92	0.52
6:a:648:A:O2'	45:i:109:SER:O	2.27	0.52
6:a:1385:A:OP1	33:h:36:ARG:NH2	2.42	0.52
5:A:252:C:O2	29:8:12:LYS:NZ	2.42	0.52
5:A:513:G:HO2'	5:A:841:C:HO2'	1.56	0.52
1:0:216:LYS:O	1:0:218:LYS:HG3	2.09	0.52
5:A:15:G:H4'	53:5:18:THR:HG22	1.92	0.52
5:A:795:A:OP1	5:A:1659:C:N4	2.43	0.52
1:0:311:LYS:CE	55:0:604:ATP:O1B	2.58	0.52
38:q:6:ARG:NH2	38:q:28:PRO:O	2.42	0.52
6:a:877:G:O2'	6:a:883:A:N1	2.37	0.52
5:A:572:C:N4	5:A:2806:U:OP2	2.41	0.52
5:A:1055:A:OP2	19:T:66:ASN:ND2	2.43	0.52
5:A:2138:U:O4	5:A:2171:G:O2'	2.27	0.52
37:p:16:ARG:NH1	37:p:19:GLU:O	2.43	0.52
38:q:73:ASN:O	38:q:76:SER:OG	2.24	0.52
22:W:46:PHE:CZ	22:W:87:ILE:HD12	2.45	0.52
5:A:846:G:O4'	10:I:54:ARG:NH2	2.43	0.51
5:A:2684:A:O3'	12:K:160:LYS:NZ	2.43	0.51
11:J:123:ASP:OD1	11:J:124:GLY:N	2.43	0.51
32:e:66:ARG:O	32:e:70:ASN:ND2	2.43	0.51
32:e:150:ILE:HB	32:e:151:ILE:HD12	1.91	0.51
44:f:99:ALA:HB2	44:f:124:LEU:CD1	2.40	0.51
6:a:421:G:O2'	6:a:436:G:N2	2.43	0.51
45:i:3:MET:O	45:i:4:THR:OG1	2.24	0.51
6:a:732:G:OP2	6:a:840:G:N2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:86:ALA:O	19:T:88:ILE:N	2.39	0.51
52:4:25:SER:OG	52:4:26:GLY:N	2.43	0.51
5:A:52:A:OP2	5:A:116:G:N1	2.43	0.51
13:M:46:THR:OG1	13:M:49:VAL:HG22	2.10	0.51
41:t:18:LYS:HB3	41:t:31:ILE:HD11	1.92	0.51
7:B:28:C:OP2	17:R:37:ASN:ND2	2.43	0.51
31:d:38:ILE:HD12	31:d:90:LEU:HD11	1.92	0.51
51:c:190:ASN:OD1	51:c:191:CYS:N	2.43	0.51
6:a:1137:U:O2'	6:a:1138:U:O5'	2.25	0.51
12:K:123:PHE:HZ	12:K:144:LEU:HD21	1.75	0.51
8:G:91:ILE:HD12	8:G:103:TYR:CD1	2.46	0.51
34:k:52:ILE:HG22	34:k:62:ARG:HD3	1.93	0.51
1:0:138:PHE:O	1:0:142:LEU:HD23	2.10	0.51
1:0:214:GLU:HA	1:0:217:ILE:HD12	1.93	0.51
1:0:264:LEU:HD23	1:0:431:ASN:OD1	2.11	0.51
5:A:2195:G:N1	5:A:2198:A:OP2	2.43	0.51
5:A:2077:C:H2'	5:A:2078:A:O4'	2.11	0.50
5:A:2557:U:O2'	5:A:2559:G:OP2	2.23	0.50
37:p:12:ILE:HG22	37:p:27:VAL:HG13	1.92	0.50
5:A:922:G:O2'	5:A:923:A:N3	2.44	0.50
5:A:1033:G:OP1	5:A:1201:G:O2'	2.29	0.50
6:a:186:U:O4	6:a:206:A:N6	2.44	0.50
8:G:146:LEU:HD11	8:G:154:ILE:HD11	1.93	0.50
15:O:48:PRO:HG2	29:8:61:LEU:HD21	1.92	0.50
16:Q:37:ALA:HA	16:Q:40:VAL:HG12	1.94	0.50
29:8:54:ASP:O	29:8:58:VAL:HG22	2.10	0.50
5:A:1031:C:O2'	5:A:1044:A:N3	2.37	0.50
5:A:1129:A:O4'	5:A:1149:U:O2'	2.27	0.50
5:A:2835:C:O2'	53:5:40:HIS:ND1	2.42	0.50
8:G:260:ARG:NH1	8:G:267:ASP:OD1	2.41	0.50
5:A:153:G:O2'	5:A:154:A:OP2	2.24	0.50
51:c:33:THR:O	51:c:40:ILE:N	2.44	0.50
5:A:618:A:OP2	5:A:2526:C:O2'	2.29	0.50
5:A:1038:C:OP1	19:T:53:ARG:NH2	2.41	0.50
49:m:59:ASN:ND2	49:m:102:ASP:OD1	2.45	0.50
51:c:206:ALA:HB3	51:c:209:ALA:HB3	1.94	0.50
5:A:2717:A:OP2	16:Q:13:ARG:NH2	2.44	0.50
6:a:744:U:O2'	47:g:91:VAL:O	2.30	0.50
7:B:40:C:OP2	52:4:2:LYS:NZ	2.45	0.50
5:A:2465:U:O2'	5:A:2467:C:OP1	2.28	0.49
51:c:131:LYS:O	51:c:135:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:127:ASN:OD1	11:J:158:THR:N	2.42	0.49
14:N:88:ARG:NH1	14:N:93:PRO:O	2.45	0.49
33:h:16:PRO:CA	43:j:48:LEU:HD11	2.42	0.49
45:i:5:ASP:OD1	45:i:79:ARG:NH1	2.39	0.49
6:a:968:A:OP1	41:t:55:ARG:NH1	2.44	0.49
6:a:1138:U:O4	34:k:9:ARG:NH1	2.46	0.49
44:f:25:VAL:N	44:f:28:GLY:O	2.46	0.49
5:A:1035:C:O2'	20:U:84:ARG:NH2	2.43	0.49
5:A:2870:A:OP2	5:A:2886:G:N1	2.43	0.49
6:a:1383:U:O2'	33:h:34:GLY:O	2.23	0.49
32:e:54:LYS:HA	32:e:194:ILE:HD13	1.93	0.49
5:A:1137:G:H21	5:A:1142:A:N6	2.02	0.49
6:a:660:U:O4	6:a:760:G:O2'	2.22	0.49
31:d:181:ILE:HG22	31:d:202:TYR:HB2	1.94	0.49
1:0:272:ILE:HD11	1:0:297:GLY:HA2	1.93	0.49
5:A:1088:C:O2'	5:A:1155:A:N1	2.37	0.49
14:N:34:ASN:O	14:N:62:ILE:HD12	2.12	0.49
19:T:48:ARG:NH2	19:T:49:ASP:OD1	2.46	0.49
38:q:69:ASP:OD1	38:q:70:THR:N	2.46	0.49
5:A:231:A:O2'	5:A:232:U:O5'	2.29	0.49
9:H:114:ASP:OD1	9:H:115:VAL:N	2.46	0.49
42:n:8:ASP:OD2	42:n:11:ARG:NH1	2.43	0.49
51:c:67:VAL:N	51:c:89:GLN:OE1	2.44	0.49
5:A:319:G:H21	5:A:325:A:H61	1.61	0.48
5:A:457:G:OP2	5:A:2433:C:O2'	2.16	0.48
5:A:2732:A:O2'	5:A:2872:G:OP1	2.27	0.48
22:W:46:PHE:CE1	22:W:87:ILE:HD12	2.49	0.48
5:A:704:U:O2	10:I:101:MET:HE1	2.13	0.48
8:G:250:TRP:O	8:G:252:LYS:N	2.44	0.48
20:U:73:VAL:HG12	20:U:73:VAL:O	2.13	0.48
4:P:65:TRP:CZ3	4:P:107:ALA:HB2	2.48	0.48
5:A:616:G:N2	5:A:2058:A:OP1	2.44	0.48
7:B:81:A:N6	7:B:90:U:H3	2.09	0.48
33:h:45:SER:OG	33:h:117:GLU:OE1	2.24	0.48
1:0:276:GLU:N	1:0:324:GLY:O	2.42	0.48
6:a:1315:G:N2	6:a:1343:A:OP2	2.37	0.48
9:H:119:THR:OG1	9:H:179:THR:HG22	2.13	0.48
6:a:528:A:OP2	49:m:61:ALA:HB1	2.13	0.48
43:j:59:THR:O	43:j:59:THR:HG22	2.13	0.48
50:r:31:LYS:N	50:r:40:VAL:O	2.47	0.48
5:A:217:G:N2	5:A:219:A:N3	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:586:C:O2'	6:a:736:A:N3	2.43	0.48
8:G:20:ASP:OD1	8:G:21:PHE:N	2.46	0.48
20:U:14:VAL:HG23	20:U:20:ILE:HD11	1.94	0.48
6:a:304:U:O2'	6:a:564:C:O2	2.31	0.48
9:H:189:ASP:O	9:H:193:LYS:N	2.47	0.48
5:A:2841:A:OP1	9:H:124:GLY:N	2.45	0.48
5:A:2135:U:O2'	5:A:2136:U:OP1	2.27	0.47
6:a:854:C:C2'	6:a:855:G:H21	2.26	0.47
9:H:174:GLY:O	9:H:176:ASN:N	2.46	0.47
14:N:79:PHE:CE1	18:S:72:VAL:HG13	2.49	0.47
31:d:29:ALA:HB1	36:o:38:LYS:HE2	1.96	0.47
47:g:23:VAL:O	47:g:27:ASN:ND2	2.46	0.47
1:0:384:VAL:CG1	55:0:603:ATP:C6	2.96	0.47
51:c:92:ILE:HD11	51:c:151:ILE:HD13	1.96	0.47
6:a:1232:G:OP1	41:t:36:ARG:NH1	2.46	0.47
6:a:1237:C:OP2	42:n:90:ARG:NH2	2.47	0.47
8:G:177:ARG:O	8:G:178:SER:OG	2.25	0.47
23:X:71:LEU:HD22	23:X:76:ASN:OD1	2.14	0.47
4:P:28:THR:O	4:P:134:ARG:NH1	2.42	0.47
5:A:1025:A:OP2	5:A:1026:C:N4	2.33	0.47
19:T:48:ARG:NH2	19:T:52:GLN:OE1	2.46	0.47
34:k:18:ILE:HG21	34:k:70:HIS:CD2	2.49	0.47
34:k:18:ILE:HG21	34:k:70:HIS:HD2	1.79	0.47
5:A:674:C:O2	5:A:684:U:O2'	2.32	0.47
5:A:1044:A:O2'	27:3:10:ARG:NH1	2.47	0.47
5:A:1451:U:H3	5:A:1632:A:H61	1.61	0.47
5:A:2195:G:O2'	5:A:2197:G:O6	2.33	0.47
6:a:946:C:O2'	6:a:1393:C:N3	2.35	0.47
6:a:1015:C:N4	6:a:1035:U:OP1	2.47	0.47
6:a:1316:G:N2	6:a:1342:G:O2'	2.43	0.47
7:B:84:U:O2'	7:B:85:U:O5'	2.32	0.47
5:A:582:G:OP1	5:A:1039:C:N4	2.47	0.47
18:S:31:HIS:ND1	18:S:44:VAL:HG22	2.29	0.47
45:i:10:MET:HG3	45:i:27:LEU:HD21	1.97	0.47
5:A:1696:C:O2'	5:A:2842:G:N2	2.48	0.47
5:A:2160:G:N2	5:A:2184:G:O2'	2.42	0.47
6:a:10:G:OP2	44:f:126:LYS:NZ	2.35	0.47
6:a:1450:G:OP1	39:u:33:LYS:NZ	2.25	0.47
7:B:38:U:O4	52:4:1:MET:N	2.45	0.47
11:J:76:THR:O	11:J:78:ARG:NH1	2.47	0.47
13:M:8:ASN:O	13:M:11:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:35:ILE:CD1	53:5:24:VAL:HG13	2.45	0.47
51:c:207:ILE:HD12	51:c:207:ILE:H	1.80	0.47
5:A:262:G:H21	5:A:666:A:H8	1.61	0.47
5:A:161:A:N3	5:A:2235:A:O2'	2.37	0.47
17:R:86:ASP:OD1	17:R:87:LYS:N	2.47	0.47
32:e:32:ALA:HB1	32:e:33:PRO:HD2	1.96	0.47
44:f:77:VAL:N	44:f:80:THR:O	2.44	0.47
51:c:90:PHE:HB3	51:c:151:ILE:HG22	1.97	0.47
5:A:1064:A:N1	5:A:1185:U:O2'	2.43	0.46
6:a:1102:U:O2'	6:a:1182:A:O2'	2.33	0.46
6:a:1281:G:O2'	6:a:1324:U:O2'	2.33	0.46
1:0:160:ASN:O	1:0:163:ASN:N	2.47	0.46
18:S:112:ILE:HG22	18:S:113:GLN:O	2.15	0.46
37:p:12:ILE:HG22	37:p:27:VAL:CG1	2.46	0.46
41:t:74:PHE:HZ	42:n:83:ILE:HD12	1.80	0.46
45:i:54:ASP:OD1	45:i:55:ASP:N	2.48	0.46
5:A:2546:U:O4'	5:A:2569:A:N6	2.48	0.46
16:Q:26:ILE:HD11	16:Q:81:ALA:HB2	1.97	0.46
46:s:66:ARG:HG2	47:g:90:MET:HE1	1.97	0.46
6:a:1026:A:O2'	6:a:1228:U:O2'	2.30	0.46
6:a:1326:U:O2'	6:a:1371:A:N3	2.39	0.46
41:t:53:ASP:OD1	41:t:56:LYS:N	2.45	0.46
13:M:34:ALA:HB2	13:M:106:ILE:HD11	1.97	0.46
22:W:13:THR:OG1	22:W:14:GLU:N	2.48	0.46
32:e:32:ALA:HB3	32:e:37:GLY:HA2	1.98	0.46
41:t:18:LYS:CB	41:t:31:ILE:HD11	2.45	0.46
5:A:499:A:N3	5:A:503:A:O2'	2.49	0.46
5:A:614:U:O2'	5:A:616:G:O5'	2.33	0.46
5:A:1357:G:N1	5:A:1367:C:OP2	2.45	0.46
32:e:8:ASN:OD1	32:e:19:LEU:HD11	2.16	0.46
32:e:65:GLU:OE2	32:e:69:ARG:NE	2.49	0.46
42:n:108:THR:OG1	42:n:109:ARG:N	2.49	0.46
1:0:227:LYS:HD2	5:A:2628:C:OP1	2.15	0.46
6:a:416:G:OP2	32:e:108:ARG:NH1	2.49	0.46
6:a:842:U:OP1	46:s:47:ARG:NH2	2.46	0.46
14:N:63:VAL:HG21	14:N:85:VAL:HG23	1.98	0.46
17:R:56:ALA:HB3	17:R:80:ILE:HG23	1.98	0.46
1:0:261:LEU:HD13	1:0:430:TYR:CD1	2.51	0.46
5:A:362:C:OP2	10:I:137:LYS:NZ	2.27	0.46
8:G:176:LEU:O	8:G:179:GLY:N	2.48	0.46
37:p:9:ASN:HA	37:p:12:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:380:LYS:NZ	55:0:603:ATP:C2	2.83	0.46
3:Z:47:ARG:NH2	5:A:2390:U:O2	2.49	0.46
14:N:63:VAL:CG1	14:N:102:VAL:HG22	2.46	0.46
47:g:43:TRP:HB2	47:g:62:ILE:HD12	1.98	0.46
6:a:1160:C:OP1	43:j:13:ARG:NH1	2.44	0.45
13:M:34:ALA:HB2	13:M:106:ILE:CD1	2.46	0.45
34:k:19:ASP:OD1	34:k:20:GLN:N	2.50	0.45
5:A:2659:A:O2'	5:A:2831:G:O2'	2.34	0.45
12:K:94:TYR:HB3	12:K:107:VAL:HG12	1.98	0.45
33:h:69:ILE:HG22	33:h:135:VAL:HG23	1.99	0.45
5:A:83:G:H21	5:A:102:A:H2	1.64	0.45
5:A:608:C:C4	5:A:619:U:O4	2.70	0.45
5:A:1153:C:O2'	5:A:1154:G:O4'	2.31	0.45
47:g:3:THR:OG1	47:g:94:GLU:O	2.33	0.45
47:g:19:LYS:O	47:g:23:VAL:HG23	2.16	0.45
5:A:2040:A:OP1	21:V:97:ASN:N	2.44	0.45
6:a:370:G:N1	6:a:373:U:OP2	2.45	0.45
11:J:85:ILE:HG22	11:J:85:ILE:O	2.16	0.45
51:c:46:THR:O	51:c:50:VAL:HG23	2.16	0.45
9:H:5:ILE:HG22	9:H:105:VAL:HG11	1.98	0.45
33:h:69:ILE:HG21	33:h:134:ALA:HB3	1.98	0.45
6:a:583:G:O2'	6:a:829:G:OP2	2.33	0.45
6:a:1013:G:N1	6:a:1048:A:N1	2.64	0.45
31:d:63:ILE:HG22	31:d:65:ILE:HG23	1.99	0.45
1:0:23:ASN:OD1	1:0:24:ARG:N	2.50	0.45
11:J:63:GLN:NE2	11:J:90:THR:O	2.49	0.45
14:N:63:VAL:CG1	14:N:102:VAL:HG13	2.46	0.45
22:W:88:ASP:N	22:W:88:ASP:OD1	2.48	0.45
5:A:620:G:O2'	5:A:1292:A:OP1	2.34	0.45
6:a:1384:G:OP2	43:j:75:THR:HG21	2.17	0.45
52:4:49:ASP:OD1	52:4:50:ILE:N	2.50	0.45
51:c:34:GLU:N	51:c:34:GLU:OE1	2.50	0.45
5:A:629:A:H5'	10:I:89:VAL:HG21	1.99	0.44
6:a:691:G:N2	35:l:39:GLY:O	2.42	0.44
8:G:2:ALA:N	8:G:20:ASP:OD2	2.51	0.44
12:K:78:GLY:O	12:K:82:GLY:N	2.48	0.44
32:e:170:ASP:OD1	32:e:171:SER:N	2.49	0.44
44:f:94:VAL:HG12	44:f:96:MET:SD	2.57	0.44
51:c:32:PHE:N	51:c:40:ILE:O	2.45	0.44
6:a:948:A:N3	6:a:1387:U:O2'	2.42	0.44
15:O:58:PHE:CD2	29:8:10:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:116:MET:HE3	33:h:120:LEU:HG	2.00	0.44
1:0:5:LEU:CD2	1:0:27:ILE:HD11	2.46	0.44
5:A:1989:C:O2'	5:A:1991:G:OP2	2.35	0.44
34:k:12:ALA:CB	34:k:18:ILE:HD12	2.48	0.44
1:0:285:ARG:NH2	55:0:604:ATP:O3'	2.51	0.44
5:A:1675:G:N2	5:A:1678:A:OP2	2.49	0.44
5:A:1982:U:O4	5:A:2583:C:N4	2.48	0.44
8:G:76:ALA:HB2	8:G:96:TYR:CE1	2.53	0.44
47:g:41:LYS:N	47:g:62:ILE:O	2.48	0.44
5:A:622:A:O2'	5:A:2046:U:OP1	2.35	0.44
6:a:181:A:H61	6:a:208:U:H2'	1.82	0.44
19:T:35:ALA:O	19:T:39:VAL:HG23	2.17	0.44
50:r:81:VAL:HG12	50:r:82:GLU:HG3	1.99	0.44
6:a:622:A:OP2	32:e:77:LYS:NZ	2.43	0.44
19:T:105:ALA:HB1	20:U:40:PHE:HZ	1.83	0.44
31:d:14:ILE:HG22	31:d:15:ILE:HG23	2.00	0.44
1:0:47:LEU:HD21	1:0:130:ILE:HG21	1.99	0.44
5:A:2776:A:H1'	12:K:63:THR:HG22	2.00	0.44
34:k:22:ALA:O	34:k:26:VAL:HG23	2.18	0.44
3:Z:40:THR:HG22	3:Z:41:GLY:H	1.83	0.43
5:A:83:G:N2	5:A:102:A:OP2	2.51	0.43
6:a:1198:G:O2'	43:j:115:ARG:NH1	2.50	0.43
18:S:62:THR:CB	18:S:75:THR:HG22	2.47	0.43
32:e:192:GLN:HA	32:e:195:VAL:HG12	2.00	0.43
37:p:56:LEU:O	37:p:60:VAL:HG23	2.18	0.43
4:P:2:LEU:C	4:P:3:LEU:HD12	2.43	0.43
5:A:2835:C:O2'	53:5:39:SER:OG	2.28	0.43
26:2:8:ASP:C	26:2:9:LEU:HD12	2.43	0.43
33:h:113:GLU:O	33:h:119:ARG:NH2	2.51	0.43
34:k:56:HIS:HD2	34:k:57:LYS:CG	2.30	0.43
40:9:25:VAL:HG22	40:9:34:GLN:HB2	2.00	0.43
44:f:106:ILE:O	44:f:125:SER:OG	2.29	0.43
5:A:576:U:OP1	5:A:604:G:N2	2.50	0.43
5:A:1379:A:O2'	5:A:1381:U:OP2	2.25	0.43
6:a:559:U:O2'	49:m:96:ARG:NH2	2.51	0.43
21:V:88:ARG:NE	21:V:94:SER:OG	2.50	0.43
32:e:119:ILE:HD12	32:e:120:LEU:N	2.34	0.43
41:t:74:PHE:CZ	42:n:83:ILE:HD12	2.54	0.43
43:j:57:THR:HG21	43:j:89:LEU:HD21	2.00	0.43
6:a:53:U:OP2	49:m:31:LYS:NZ	2.49	0.43
6:a:262:G:O3'	50:r:73:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:412:G:OP1	32:e:115:ASN:ND2	2.43	0.43
14:N:61:VAL:HG23	14:N:87:ILE:HD13	2.01	0.43
15:O:86:GLU:O	15:O:89:THR:HG22	2.18	0.43
5:A:375:A:O2'	5:A:377:U:OP2	2.18	0.43
5:A:1942:U:O2'	5:A:1943:A:O5'	2.36	0.43
5:A:2715:G:OP1	5:A:2740:A:N6	2.51	0.43
13:M:57:VAL:HB	13:M:125:VAL:HG22	1.99	0.43
35:l:68:GLU:HG3	35:l:99:ALA:HB1	2.00	0.43
6:a:285:C:OP1	50:r:47:LYS:NZ	2.38	0.43
5:A:2496:A:N6	5:A:2508:G:O2'	2.51	0.43
13:M:5:PHE:O	19:T:64:ARG:NH2	2.44	0.43
24:Y:29:ALA:HB2	24:Y:89:ILE:HB	2.01	0.43
26:2:45:THR:O	26:2:49:THR:HG23	2.17	0.43
32:e:54:LYS:CA	32:e:194:ILE:HD13	2.49	0.43
32:e:95:ASP:OD1	32:e:96:ALA:N	2.51	0.43
43:j:65:VAL:C	43:j:66:LEU:HD12	2.43	0.43
6:a:753:U:O3'	6:a:844:G:N2	2.52	0.43
8:G:142:HIS:HA	8:G:155:ALA:HB3	2.00	0.43
50:r:17:ASP:OD2	50:r:57:LEU:N	2.52	0.43
3:Z:23:ASP:OD1	3:Z:24:SER:N	2.50	0.43
6:a:797:U:N3	6:a:800:A:OP2	2.46	0.43
7:B:87:C:O2'	7:B:88:G:OP1	2.34	0.43
14:N:64:ARG:HB2	14:N:79:PHE:CD2	2.54	0.43
1:0:3:ILE:HG23	1:0:28:TYR:CE1	2.54	0.43
1:0:364:ILE:HD13	1:0:400:LEU:HD22	2.01	0.43
6:a:51:A:O2'	6:a:368:G:N2	2.50	0.43
43:j:57:THR:HG23	43:j:59:THR:OG1	2.18	0.43
49:m:14:SER:OG	49:m:15:LYS:N	2.51	0.43
5:A:1452:C:H3'	5:A:1453:G:H21	1.84	0.42
6:a:587:G:O3'	37:p:54:ARG:NH1	2.45	0.42
6:a:1324:U:OP2	41:t:6:LYS:N	2.52	0.42
12:K:107:VAL:HG23	12:K:107:VAL:O	2.19	0.42
45:i:118:ALA:HB1	45:i:123:VAL:O	2.18	0.42
1:0:360:ASN:OD1	1:0:361:GLU:N	2.52	0.42
3:Z:34:ALA:N	3:Z:37:GLN:OE1	2.51	0.42
5:A:1845:U:O2'	8:G:153:GLN:O	2.24	0.42
5:A:2432:G:O2'	5:A:2438:A:N6	2.52	0.42
12:K:86:VAL:C	12:K:87:LEU:HD12	2.44	0.42
16:Q:48:ILE:HG21	16:Q:100:TYR:CD1	2.54	0.42
41:t:32:LYS:HG2	41:t:50:ALA:HB3	2.02	0.42
49:m:26:LYS:HD2	49:m:74:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:47:ARG:HG2	3:Z:66:THR:HG22	2.01	0.42
5:A:1854:U:OP2	8:G:221:ARG:NE	2.52	0.42
6:a:948:A:O2'	33:h:95:ARG:NH2	2.50	0.42
31:d:119:ILE:HD11	31:d:197:VAL:HB	2.01	0.42
5:A:1822:C:H2'	5:A:1823:U:O4'	2.19	0.42
5:A:2160:G:HO2'	5:A:2161:A:P	2.41	0.42
5:A:2457:A:HO2'	5:A:2458:U:P	2.42	0.42
6:a:1119:C:OP1	31:d:171:THR:OG1	2.28	0.42
6:a:1331:C:O2	41:t:36:ARG:NH2	2.53	0.42
31:d:11:ARG:NH2	31:d:174:LEU:O	2.52	0.42
34:k:52:ILE:HG22	34:k:62:ARG:CD	2.49	0.42
1:0:3:ILE:HG22	1:0:5:LEU:H	1.84	0.42
33:h:47:PHE:HA	33:h:50:VAL:HG12	2.02	0.42
2:D:12:G:N3	5:A:1950:U:O2'	2.52	0.42
5:A:1072:A:H2'	5:A:1073:A:H8	1.83	0.42
6:a:956:A:O2'	6:a:1344:A:O2'	2.33	0.42
8:G:76:ALA:HB2	8:G:96:TYR:CD1	2.55	0.42
23:X:48:THR:HG22	23:X:49:GLN:N	2.35	0.42
31:d:107:LYS:HD3	31:d:110:LEU:HD22	2.02	0.42
34:k:90:LEU:HD11	34:k:92:LEU:HD12	2.01	0.42
3:Z:58:ASN:HB3	3:Z:71:ILE:HG22	2.02	0.42
5:A:2333:U:O2	5:A:2338:A:N6	2.52	0.42
5:A:2558:A:H61	5:A:2689:A:H61	1.66	0.42
6:a:74:G:N2	6:a:95:A:OP2	2.46	0.42
6:a:1261:A:OP1	43:j:71:GLY:N	2.45	0.42
34:k:12:ALA:HB3	34:k:18:ILE:HD12	2.01	0.42
5:A:418:G:O2'	5:A:446:G:O6	2.28	0.42
5:A:2388:A:OP1	29:8:27:ALA:N	2.51	0.42
5:A:2821:U:N3	5:A:2823:G:OP1	2.53	0.42
12:K:37:LEU:HD13	12:K:68:THR:HG23	2.02	0.42
18:S:94:VAL:HG12	18:S:96:ARG:H	1.85	0.42
5:A:247:A:OP2	29:8:8:ARG:NH2	2.46	0.42
5:A:1891:U:OP1	5:A:2437:G:O2'	2.36	0.42
7:B:22:G:H1'	7:B:25:A:H61	1.85	0.42
32:e:138:THR:OG1	32:e:174:GLY:O	2.30	0.42
37:p:76:GLN:OE1	37:p:79:ARG:NH2	2.47	0.42
1:0:40:GLY:HA2	55:0:603:ATP:H3'	2.02	0.41
5:A:1304:G:OP2	53:5:17:ARG:NE	2.40	0.41
11:J:117:VAL:HG12	11:J:176:PRO:HG2	2.01	0.41
12:K:95:ARG:NH2	12:K:97:GLN:OE1	2.52	0.41
15:O:69:ILE:HD12	15:O:70:ASN:CG	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:6:ILE:HA	26:2:9:LEU:HD13	2.02	0.41
45:i:10:MET:CG	45:i:27:LEU:HD21	2.50	0.41
5:A:160:G:H21	5:A:168:A:H2	1.68	0.41
6:a:747:C:OP1	47:g:2:ARG:NH2	2.46	0.41
18:S:16:ARG:NH2	18:S:80:THR:O	2.53	0.41
39:u:4:ILE:HD12	39:u:8:ILE:CG2	2.49	0.41
5:A:1456:U:O2'	5:A:1457:U:O5'	2.25	0.41
5:A:1851:G:OP2	8:G:53:HIS:ND1	2.53	0.41
6:a:930:U:O2'	6:a:1093:G:O2'	2.03	0.41
6:a:1047:G:O2'	6:a:1048:A:O4'	2.37	0.41
12:K:17:VAL:HG11	12:K:50:ILE:CD1	2.50	0.41
14:N:64:ARG:HB2	14:N:79:PHE:HD2	1.86	0.41
46:s:39:SER:OG	46:s:43:LYS:N	2.43	0.41
5:A:963:A:N3	7:B:78:U:O2'	2.52	0.41
5:A:1101:A:H62	5:A:1130:A:H2'	1.84	0.41
5:A:1826:G:OP1	8:G:260:ARG:NE	2.47	0.41
6:a:572:U:C2	50:r:35:LEU:HD21	2.55	0.41
16:Q:45:GLU:OE2	16:Q:101:THR:HG22	2.20	0.41
27:3:11:SER:OG	27:3:12:VAL:N	2.53	0.41
31:d:105:ILE:O	31:d:105:ILE:HG23	2.20	0.41
37:p:39:VAL:O	37:p:43:LEU:HD13	2.20	0.41
42:n:55:ARG:O	42:n:59:VAL:HG23	2.20	0.41
42:n:69:LEU:O	42:n:73:THR:HG23	2.21	0.41
14:N:63:VAL:HG21	14:N:85:VAL:CG2	2.50	0.41
5:A:1449:A:H8	5:A:1634:A:H62	1.69	0.41
6:a:919:A:OP1	49:m:18:LYS:NZ	2.52	0.41
10:I:101:MET:O	10:I:106:ARG:NH2	2.44	0.41
13:M:7:ALA:H	13:M:46:THR:HG21	1.85	0.41
19:T:106:PHE:O	19:T:110:VAL:HG23	2.21	0.41
23:X:33:VAL:O	23:X:63:ILE:N	2.45	0.41
31:d:119:ILE:HG22	31:d:132:VAL:CG1	2.50	0.41
1:0:384:VAL:HG13	55:0:603:ATP:C6	2.56	0.41
2:D:22:A:HO2'	2:D:23:G:P	2.43	0.41
5:A:1044:A:OP2	5:A:1198:G:N1	2.45	0.41
14:N:71:ARG:NE	14:N:77:ILE:HD11	2.35	0.41
15:O:97:VAL:HG22	15:O:102:VAL:HG23	2.01	0.41
25:1:36:VAL:HG12	25:1:49:VAL:HG12	2.02	0.41
34:k:57:LYS:HB2	34:k:58:TYR:H	1.68	0.41
47:g:30:LEU:HD21	47:g:76:PHE:CD1	2.56	0.41
5:A:526:A:H3'	5:A:527:G:H5''	2.03	0.41
6:a:148:G:H1	6:a:174:A:H61	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:446:G:N2	6:a:504:G:N7	2.42	0.41
6:a:1047:G:N2	6:a:1048:A:N3	2.68	0.41
9:H:10:ILE:HD13	18:S:6:LEU:HD13	2.03	0.41
11:J:50:LEU:O	11:J:54:VAL:HG23	2.21	0.41
15:O:69:ILE:HD12	15:O:70:ASN:N	2.35	0.41
15:O:123:VAL:HG12	15:O:124:LYS:N	2.36	0.41
27:3:19:GLN:O	27:3:23:VAL:HG23	2.21	0.41
1:0:44:THR:OG1	55:0:603:ATP:O2B	2.39	0.41
5:A:273:A:OP2	5:A:297:G:N1	2.47	0.41
16:Q:102:ARG:NH2	16:Q:122:VAL:OXT	2.54	0.41
6:a:185:U:O3'	39:u:76:SER:OG	2.38	0.40
6:a:1251:U:O4	33:h:109:ARG:NE	2.53	0.40
21:V:47:ILE:HG23	21:V:105:ILE:CD1	2.50	0.40
24:Y:76:ASP:OD1	24:Y:77:TYR:N	2.54	0.40
32:e:151:ILE:O	32:e:155:VAL:HG23	2.20	0.40
34:k:56:HIS:CD2	34:k:57:LYS:HG3	2.53	0.40
45:i:80:ILE:HG22	45:i:81:SER:N	2.36	0.40
47:g:33:GLU:HB3	47:g:72:ALA:HB2	2.02	0.40
6:a:1320:G:OP2	42:n:98:ARG:NH2	2.48	0.40
12:K:10:ASP:OD1	12:K:11:ILE:N	2.54	0.40
45:i:15:ARG:NH2	45:i:77:LEU:O	2.51	0.40
45:i:110:GLU:OE1	45:i:121:ARG:NH1	2.54	0.40
1:0:227:LYS:NZ	5:A:2628:C:OP1	2.52	0.40
4:P:58:MET:SD	4:P:109:VAL:HG11	2.61	0.40
6:a:854:C:H2'	6:a:855:G:H21	1.87	0.40
11:J:122:PHE:CE2	11:J:166:ALA:HB3	2.57	0.40
27:3:52:HIS:CD2	27:3:53:LEU:HD12	2.56	0.40
47:g:70:ASN:OD1	47:g:72:ALA:HB3	2.20	0.40
4:P:54:MET:SD	4:P:118:LEU:HD23	2.61	0.40
5:A:566:U:H2'	5:A:567:G:C8	2.56	0.40
5:A:826:A:OP1	8:G:217:ARG:NH1	2.53	0.40
39:u:7:ALA:O	39:u:10:ARG:N	2.54	0.40
1:0:18:LEU:HD21	1:0:21:ASN:HB2	2.04	0.40
5:A:1038:C:O2'	20:U:10:LYS:NZ	2.46	0.40
6:a:89:U:O2'	6:a:90:C:O4'	2.34	0.40
11:J:117:VAL:HG22	11:J:118:SER:H	1.87	0.40
42:n:22:ILE:CG2	42:n:25:ILE:HD12	2.50	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	463/546 (85%)	420 (91%)	43 (9%)	0	100	100
3	Z	74/94 (79%)	68 (92%)	6 (8%)	0	100	100
4	P	133/144 (92%)	120 (90%)	13 (10%)	0	100	100
8	G	271/277 (98%)	245 (90%)	26 (10%)	0	100	100
9	H	214/220 (97%)	193 (90%)	21 (10%)	0	100	100
10	I	202/207 (98%)	180 (89%)	22 (11%)	0	100	100
11	J	173/179 (97%)	150 (87%)	23 (13%)	0	100	100
12	K	162/178 (91%)	155 (96%)	7 (4%)	0	100	100
13	M	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
14	N	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
15	O	143/146 (98%)	131 (92%)	12 (8%)	0	100	100
16	Q	118/122 (97%)	112 (95%)	6 (5%)	0	100	100
17	R	116/119 (98%)	105 (90%)	11 (10%)	0	100	100
18	S	112/116 (97%)	96 (86%)	16 (14%)	0	100	100
19	T	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
20	U	99/102 (97%)	89 (90%)	10 (10%)	0	100	100
21	V	109/117 (93%)	106 (97%)	3 (3%)	0	100	100
22	W	87/91 (96%)	78 (90%)	9 (10%)	0	100	100
23	X	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
24	Y	92/217 (42%)	81 (88%)	11 (12%)	0	100	100
25	1	58/62 (94%)	51 (88%)	7 (12%)	0	100	100
26	2	62/69 (90%)	57 (92%)	5 (8%)	0	100	100
27	3	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
28	6	45/49 (92%)	38 (84%)	7 (16%)	0	100	100
29	8	62/66 (94%)	56 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	7	40/45 (89%)	39 (98%)	1 (2%)	0	100	100
31	d	206/217 (95%)	185 (90%)	21 (10%)	0	100	100
32	e	197/200 (98%)	173 (88%)	24 (12%)	0	100	100
33	h	134/156 (86%)	121 (90%)	13 (10%)	0	100	100
34	k	98/102 (96%)	85 (87%)	13 (13%)	0	100	100
35	l	116/129 (90%)	107 (92%)	9 (8%)	0	100	100
36	o	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
37	p	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
38	q	88/91 (97%)	79 (90%)	9 (10%)	0	100	100
39	u	78/83 (94%)	73 (94%)	5 (6%)	0	100	100
40	9	34/37 (92%)	30 (88%)	4 (12%)	0	100	100
41	t	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
42	n	114/121 (94%)	96 (84%)	18 (16%)	0	100	100
43	j	125/132 (95%)	118 (94%)	7 (6%)	0	100	100
44	f	154/166 (93%)	142 (92%)	12 (8%)	0	100	100
45	i	129/132 (98%)	117 (91%)	12 (9%)	0	100	100
46	s	61/80 (76%)	54 (88%)	7 (12%)	0	100	100
47	g	91/98 (93%)	79 (87%)	12 (13%)	0	100	100
49	m	133/137 (97%)	111 (84%)	22 (16%)	0	100	100
50	r	77/87 (88%)	67 (87%)	10 (13%)	0	100	100
51	c	219/255 (86%)	199 (91%)	20 (9%)	0	100	100
52	4	53/84 (63%)	47 (89%)	6 (11%)	0	100	100
53	5	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
All	All	5737/6320 (91%)	5190 (90%)	547 (10%)	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	423/500 (85%)	421 (100%)	2 (0%)	81	85
3	Z	59/75 (79%)	59 (100%)	0	100	100
4	P	112/119 (94%)	112 (100%)	0	100	100
8	G	220/224 (98%)	219 (100%)	1 (0%)	81	85
9	H	174/177 (98%)	174 (100%)	0	100	100
10	I	168/169 (99%)	168 (100%)	0	100	100
11	J	154/158 (98%)	154 (100%)	0	100	100
12	K	144/155 (93%)	144 (100%)	0	100	100
13	M	121/123 (98%)	121 (100%)	0	100	100
14	N	100/100 (100%)	100 (100%)	0	100	100
15	O	111/112 (99%)	111 (100%)	0	100	100
16	Q	101/102 (99%)	101 (100%)	0	100	100
17	R	94/95 (99%)	94 (100%)	0	100	100
18	S	100/102 (98%)	100 (100%)	0	100	100
19	T	96/98 (98%)	95 (99%)	1 (1%)	68	79
20	U	86/86 (100%)	86 (100%)	0	100	100
21	V	90/94 (96%)	90 (100%)	0	100	100
22	W	80/82 (98%)	80 (100%)	0	100	100
23	X	84/90 (93%)	84 (100%)	0	100	100
24	Y	83/190 (44%)	83 (100%)	0	100	100
25	1	50/52 (96%)	50 (100%)	0	100	100
26	2	58/62 (94%)	58 (100%)	0	100	100
27	3	51/53 (96%)	51 (100%)	0	100	100
28	6	45/47 (96%)	45 (100%)	0	100	100
29	8	55/57 (96%)	55 (100%)	0	100	100
30	7	38/40 (95%)	38 (100%)	0	100	100
31	d	169/175 (97%)	169 (100%)	0	100	100
32	e	174/175 (99%)	174 (100%)	0	100	100
33	h	117/132 (89%)	117 (100%)	0	100	100
34	k	90/91 (99%)	89 (99%)	1 (1%)	65	78
35	l	94/104 (90%)	94 (100%)	0	100	100
36	o	52/53 (98%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	p	80/81 (99%)	80 (100%)	0	100	100
38	q	76/77 (99%)	76 (100%)	0	100	100
39	u	67/69 (97%)	67 (100%)	0	100	100
40	9	35/35 (100%)	35 (100%)	0	100	100
41	t	70/80 (88%)	70 (100%)	0	100	100
42	n	100/104 (96%)	100 (100%)	0	100	100
43	j	105/109 (96%)	105 (100%)	0	100	100
44	f	122/131 (93%)	122 (100%)	0	100	100
45	i	112/113 (99%)	112 (100%)	0	100	100
46	s	56/68 (82%)	56 (100%)	0	100	100
47	g	81/86 (94%)	81 (100%)	0	100	100
49	m	117/119 (98%)	117 (100%)	0	100	100
50	r	74/82 (90%)	74 (100%)	0	100	100
51	c	192/221 (87%)	192 (100%)	0	100	100
52	4	55/75 (73%)	55 (100%)	0	100	100
53	5	48/50 (96%)	48 (100%)	0	100	100
All	All	4983/5392 (92%)	4978 (100%)	5 (0%)	87	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	73	LEU
1	0	375	ARG
8	G	14	ARG
19	T	92	ARG
34	k	57	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	12	HIS
1	0	29	GLN
1	0	66	HIS
8	G	45	ASN
10	I	30	ASN

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Mol	Chain	Res	Type
10	I	162	ASN
15	O	27	ASN
18	S	79	HIS
24	Y	84	ASN
27	3	40	ASN
27	3	48	ASN
28	6	4	ASN
31	d	44	ASN
31	d	68	HIS
31	d	88	ASN
32	e	39	ASN
33	h	18	HIS
34	k	56	HIS
36	o	31	HIS
37	p	18	HIS
41	t	57	HIS
42	n	31	GLN
43	j	62	ASN
47	g	53	ASN
49	m	77	ASN
51	c	18	HIS
51	c	94	GLN
53	5	14	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	72/76 (94%)	19 (26%)	1 (1%)
48	b	7/15 (46%)	0	0
5	A	2912/2923 (99%)	532 (18%)	15 (0%)
6	a	1536/1551 (99%)	288 (18%)	0
7	B	112/115 (97%)	16 (14%)	0
All	All	4639/4680 (99%)	855 (18%)	16 (0%)

All (855) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	8	U
2	D	9	G
2	D	13	C
2	D	19	G

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Mol	Chain	Res	Type
2	D	20	G
2	D	21	U
2	D	22	A
2	D	23	G
2	D	32	G
2	D	45	A
2	D	47	G
2	D	48	U
2	D	49	C
2	D	54	G
2	D	59	A
2	D	60	A
2	D	71	G
2	D	72	C
2	D	73	A
5	A	13	A
5	A	15	G
5	A	23	G
5	A	35	G
5	A	36	G
5	A	61	A
5	A	63	U
5	A	64	A
5	A	71	A
5	A	75	G
5	A	88	G
5	A	96	G
5	A	99	U
5	A	117	A
5	A	118	A
5	A	119	U
5	A	122	G
5	A	130	A
5	A	133	A
5	A	154	A
5	A	155	U
5	A	157	U
5	A	164	A
5	A	165	C
5	A	167	U
5	A	168	A
5	A	169	G

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Mol	Chain	Res	Type
5	A	175	C
5	A	176	A
5	A	177	G
5	A	184	C
5	A	185	A
5	A	199	A
5	A	202	A
5	A	207	A
5	A	218	G
5	A	219	A
5	A	224	A
5	A	225	A
5	A	228	A
5	A	229	A
5	A	231	A
5	A	233	U
5	A	236	A
5	A	251	G
5	A	253	G
5	A	255	G
5	A	268	A
5	A	270	C
5	A	281	A
5	A	283	G
5	A	284	C
5	A	285	U
5	A	286	U
5	A	287	G
5	A	299	U
5	A	302	A
5	A	311	U
5	A	313	U
5	A	314	A
5	A	321	U
5	A	354	A
5	A	360	A
5	A	367	A
5	A	373	A
5	A	388	A
5	A	389	A
5	A	403	U
5	A	404	U

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Mol	Chain	Res	Type
5	A	410	G
5	A	415	U
5	A	418	G
5	A	419	U
5	A	426	G
5	A	431	C
5	A	432	G
5	A	450	C
5	A	457	G
5	A	458	A
5	A	459	C
5	A	470	G
5	A	476	A
5	A	493	A
5	A	494	U
5	A	497	U
5	A	502	C
5	A	503	A
5	A	510	U
5	A	527	G
5	A	541	G
5	A	550	A
5	A	553	A
5	A	554	C
5	A	567	G
5	A	572	C
5	A	575	G
5	A	576	U
5	A	577	A
5	A	578	G
5	A	590	U
5	A	591	A
5	A	592	A
5	A	593	U
5	A	594	G
5	A	606	G
5	A	615	A
5	A	616	G
5	A	617	A
5	A	618	A
5	A	626	G
5	A	630	G

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Mol	Chain	Res	Type
5	A	646	A
5	A	658	A
5	A	659	A
5	A	666	A
5	A	667	G
5	A	679	G
5	A	681	G
5	A	682	A
5	A	683	G
5	A	690	U
5	A	691	A
5	A	699	U
5	A	700	A
5	A	727	G
5	A	731	U
5	A	763	A
5	A	764	C
5	A	775	A
5	A	783	G
5	A	792	U
5	A	793	G
5	A	807	U
5	A	813	G
5	A	816	G
5	A	819	A
5	A	820	G
5	A	827	A
5	A	829	U
5	A	830	U
5	A	835	U
5	A	837	G
5	A	850	G
5	A	854	G
5	A	857	C
5	A	872	U
5	A	873	U
5	A	904	G
5	A	911	A
5	A	919	G
5	A	921	C
5	A	923	A
5	A	924	G

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Mol	Chain	Res	Type
5	A	930	C
5	A	936	G
5	A	940	U
5	A	941	A
5	A	943	C
5	A	944	G
5	A	945	A
5	A	955	A
5	A	959	C
5	A	960	C
5	A	970	U
5	A	985	A
5	A	989	A
5	A	990	G
5	A	1001	A
5	A	1005	G
5	A	1017	A
5	A	1018	A
5	A	1026	C
5	A	1027	A
5	A	1029	C
5	A	1040	A
5	A	1041	G
5	A	1049	C
5	A	1056	U
5	A	1057	A
5	A	1066	G
5	A	1069	G
5	A	1070	A
5	A	1077	U
5	A	1083	G
5	A	1085	U
5	A	1089	C
5	A	1091	G
5	A	1101	A
5	A	1104	U
5	A	1105	U
5	A	1106	G
5	A	1110	U
5	A	1113	A
5	A	1114	A
5	A	1115	G

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Mol	Chain	Res	Type
5	A	1117	A
5	A	1118	G
5	A	1128	A
5	A	1131	G
5	A	1132	A
5	A	1134	U
5	A	1139	A
5	A	1140	A
5	A	1141	U
5	A	1149	U
5	A	1155	A
5	A	1156	G
5	A	1160	C
5	A	1163	U
5	A	1166	G
5	A	1174	U
5	A	1176	U
5	A	1177	A
5	A	1178	C
5	A	1179	C
5	A	1186	A
5	A	1195	A
5	A	1216	U
5	A	1217	U
5	A	1218	G
5	A	1249	U
5	A	1250	G
5	A	1276	G
5	A	1282	A
5	A	1285	A
5	A	1286	G
5	A	1294	G
5	A	1303	A
5	A	1309	G
5	A	1310	A
5	A	1318	G
5	A	1337	A
5	A	1338	U
5	A	1339	U
5	A	1342	C
5	A	1355	A
5	A	1358	A

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Mol	Chain	Res	Type
5	A	1366	U
5	A	1378	U
5	A	1382	C
5	A	1387	C
5	A	1402	A
5	A	1405	G
5	A	1416	U
5	A	1432	A
5	A	1440	A
5	A	1449	A
5	A	1451	U
5	A	1452	C
5	A	1454	U
5	A	1455	U
5	A	1456	U
5	A	1457	U
5	A	1458	A
5	A	1459	A
5	A	1463	A
5	A	1464	U
5	A	1468	G
5	A	1472	C
5	A	1481	A
5	A	1488	A
5	A	1490	G
5	A	1494	G
5	A	1496	G
5	A	1497	A
5	A	1500	G
5	A	1504	U
5	A	1505	G
5	A	1511	C
5	A	1526	G
5	A	1527	A
5	A	1532	U
5	A	1533	A
5	A	1534	G
5	A	1535	G
5	A	1536	C
5	A	1537	A
5	A	1552	U
5	A	1553	A

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Mol	Chain	Res	Type
5	A	1560	A
5	A	1567	A
5	A	1568	U
5	A	1574	G
5	A	1582	U
5	A	1583	G
5	A	1591	G
5	A	1592	A
5	A	1594	U
5	A	1606	C
5	A	1613	G
5	A	1616	A
5	A	1618	A
5	A	1625	U
5	A	1631	G
5	A	1634	A
5	A	1641	G
5	A	1651	C
5	A	1652	A
5	A	1653	A
5	A	1654	A
5	A	1660	A
5	A	1670	A
5	A	1683	U
5	A	1690	A
5	A	1691	G
5	A	1692	C
5	A	1716	C
5	A	1718	G
5	A	1719	C
5	A	1721	A
5	A	1738	C
5	A	1740	G
5	A	1742	A
5	A	1747	G
5	A	1759	G
5	A	1764	A
5	A	1765	A
5	A	1768	C
5	A	1772	G
5	A	1781	C
5	A	1783	G

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Mol	Chain	Res	Type
5	A	1790	G
5	A	1791	G
5	A	1800	A
5	A	1808	U
5	A	1809	C
5	A	1811	A
5	A	1827	C
5	A	1828	U
5	A	1829	A
5	A	1835	U
5	A	1836	A
5	A	1839	G
5	A	1843	U
5	A	1846	A
5	A	1856	A
5	A	1860	C
5	A	1865	C
5	A	1872	G
5	A	1875	A
5	A	1891	U
5	A	1893	A
5	A	1896	U
5	A	1897	U
5	A	1899	U
5	A	1907	U
5	A	1909	C
5	A	1926	A
5	A	1930	G
5	A	1933	G
5	A	1934	G
5	A	1939	A
5	A	1940	A
5	A	1943	A
5	A	1954	A
5	A	1956	G
5	A	1957	G
5	A	1958	U
5	A	1963	A
5	A	1964	A
5	A	1965	A
5	A	1967	U
5	A	1968	C

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Mol	Chain	Res	Type
5	A	1970	U
5	A	1982	U
5	A	1988	C
5	A	1994	C
5	A	1997	A
5	A	1998	A
5	A	1999	G
5	A	2018	U
5	A	2020	U
5	A	2023	C
5	A	2040	A
5	A	2057	A
5	A	2058	A
5	A	2059	G
5	A	2060	A
5	A	2070	C
5	A	2076	A
5	A	2078	A
5	A	2082	C
5	A	2083	G
5	A	2087	A
5	A	2088	G
5	A	2089	A
5	A	2096	G
5	A	2119	U
5	A	2120	G
5	A	2135	U
5	A	2136	U
5	A	2139	A
5	A	2143	G
5	A	2144	A
5	A	2145	U
5	A	2153	A
5	A	2175	G
5	A	2176	C
5	A	2180	C
5	A	2184	G
5	A	2185	A
5	A	2186	G
5	A	2187	G
5	A	2199	U
5	A	2203	A

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Mol	Chain	Res	Type
5	A	2217	G
5	A	2221	U
5	A	2225	A
5	A	2231	C
5	A	2237	U
5	A	2238	U
5	A	2239	A
5	A	2240	U
5	A	2241	C
5	A	2251	G
5	A	2252	A
5	A	2254	A
5	A	2265	G
5	A	2266	G
5	A	2273	G
5	A	2290	C
5	A	2293	A
5	A	2295	A
5	A	2305	A
5	A	2310	C
5	A	2314	A
5	A	2326	G
5	A	2333	U
5	A	2334	G
5	A	2335	G
5	A	2336	A
5	A	2337	A
5	A	2338	A
5	A	2347	A
5	A	2352	G
5	A	2361	U
5	A	2362	A
5	A	2374	C
5	A	2377	C
5	A	2381	A
5	A	2385	A
5	A	2410	G
5	A	2412	C
5	A	2415	A
5	A	2418	G
5	A	2433	C
5	A	2438	A

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Mol	Chain	Res	Type
5	A	2446	U
5	A	2449	C
5	A	2450	U
5	A	2452	A
5	A	2456	G
5	A	2457	A
5	A	2458	U
5	A	2459	A
5	A	2468	C
5	A	2472	G
5	A	2475	A
5	A	2478	A
5	A	2492	C
5	A	2495	A
5	A	2497	G
5	A	2503	A
5	A	2505	A
5	A	2511	G
5	A	2514	G
5	A	2521	G
5	A	2529	G
5	A	2531	U
5	A	2545	A
5	A	2546	U
5	A	2547	C
5	A	2556	G
5	A	2557	U
5	A	2562	G
5	A	2582	U
5	A	2593	A
5	A	2594	G
5	A	2601	G
5	A	2605	G
5	A	2609	G
5	A	2629	A
5	A	2637	C
5	A	2640	U
5	A	2642	U
5	A	2657	G
5	A	2663	U
5	A	2690	G
5	A	2700	G

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Mol	Chain	Res	Type
5	A	2709	U
5	A	2712	G
5	A	2716	U
5	A	2718	C
5	A	2727	G
5	A	2741	G
5	A	2753	U
5	A	2756	G
5	A	2760	A
5	A	2762	G
5	A	2771	G
5	A	2784	A
5	A	2791	A
5	A	2792	A
5	A	2793	G
5	A	2805	A
5	A	2806	U
5	A	2820	U
5	A	2822	C
5	A	2823	G
5	A	2824	G
5	A	2827	A
5	A	2838	C
5	A	2840	A
5	A	2844	U
5	A	2845	G
5	A	2847	U
5	A	2853	U
5	A	2854	A
5	A	2863	G
5	A	2877	G
5	A	2886	G
5	A	2887	G
5	A	2892	G
5	A	2894	C
5	A	2899	A
5	A	2900	C
5	A	2903	A
5	A	2905	C
5	A	2906	G
5	A	2907	A
5	A	2911	A

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Mol	Chain	Res	Type
5	A	2913	G
6	a	8	G
6	a	10	G
6	a	33	A
6	a	40	G
6	a	45	G
6	a	48	C
6	a	49	C
6	a	50	U
6	a	51	A
6	a	52	A
6	a	59	C
6	a	82	G
6	a	83	C
6	a	84	U
6	a	85	U
6	a	87	C
6	a	89	U
6	a	90	C
6	a	91	U
6	a	92	C
6	a	93	U
6	a	94	G
6	a	97	G
6	a	107	G
6	a	108	A
6	a	120	C
6	a	121	A
6	a	129	A
6	a	130	A
6	a	131	C
6	a	134	A
6	a	136	C
6	a	138	A
6	a	142	G
6	a	144	C
6	a	154	U
6	a	156	C
6	a	159	G
6	a	163	C
6	a	164	C
6	a	167	A

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Mol	Chain	Res	Type
6	a	173	U
6	a	174	A
6	a	182	A
6	a	183	U
6	a	189	G
6	a	196	A
6	a	198	G
6	a	204	A
6	a	212	A
6	a	213	G
6	a	216	G
6	a	221	U
6	a	222	G
6	a	234	A
6	a	249	G
6	a	253	U
6	a	255	G
6	a	259	G
6	a	261	U
6	a	267	G
6	a	270	A
6	a	274	G
6	a	275	C
6	a	281	A
6	a	288	C
6	a	297	G
6	a	314	A
6	a	329	A
6	a	336	C
6	a	337	A
6	a	338	C
6	a	344	A
6	a	353	C
6	a	355	G
6	a	360	C
6	a	361	A
6	a	362	G
6	a	364	A
6	a	375	U
6	a	380	C
6	a	400	G
6	a	405	A

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Mol	Chain	Res	Type
6	a	406	C
6	a	414	G
6	a	419	A
6	a	420	U
6	a	421	G
6	a	424	G
6	a	429	U
6	a	430	C
6	a	432	G
6	a	436	G
6	a	437	U
6	a	439	A
6	a	441	A
6	a	448	U
6	a	456	A
6	a	459	A
6	a	460	A
6	a	461	C
6	a	463	U
6	a	466	G
6	a	471	A
6	a	472	G
6	a	476	C
6	a	490	A
6	a	493	G
6	a	499	A
6	a	505	A
6	a	517	A
6	a	518	A
6	a	526	C
6	a	529	G
6	a	532	G
6	a	535	G
6	a	540	A
6	a	555	A
6	a	567	A
6	a	570	U
6	a	572	U
6	a	578	G
6	a	580	A
6	a	581	A
6	a	584	C

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Mol	Chain	Res	Type
6	a	585	G
6	a	589	G
6	a	623	C
6	a	624	G
6	a	626	C
6	a	631	C
6	a	641	U
6	a	642	C
6	a	661	U
6	a	664	G
6	a	668	A
6	a	669	G
6	a	695	A
6	a	710	A
6	a	728	C
6	a	731	U
6	a	742	A
6	a	757	A
6	a	761	A
6	a	763	G
6	a	785	A
6	a	801	U
6	a	802	A
6	a	807	G
6	a	817	G
6	a	825	C
6	a	836	A
6	a	844	G
6	a	851	U
6	a	854	C
6	a	855	G
6	a	856	C
6	a	861	U
6	a	863	G
6	a	869	C
6	a	880	U
6	a	882	A
6	a	886	A
6	a	895	G
6	a	899	A
6	a	910	A
6	a	932	G

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Mol	Chain	Res	Type
6	a	936	G
6	a	944	C
6	a	945	A
6	a	970	U
6	a	976	G
6	a	977	C
6	a	979	A
6	a	981	G
6	a	982	C
6	a	985	A
6	a	986	G
6	a	987	A
6	a	992	U
6	a	999	U
6	a	1002	U
6	a	1003	G
6	a	1004	A
6	a	1012	U
6	a	1014	A
6	a	1016	A
6	a	1025	G
6	a	1028	A
6	a	1031	G
6	a	1033	C
6	a	1034	U
6	a	1035	U
6	a	1036	C
6	a	1037	C
6	a	1047	G
6	a	1055	G
6	a	1057	C
6	a	1058	A
6	a	1077	U
6	a	1078	C
6	a	1097	U
6	a	1106	G
6	a	1113	A
6	a	1116	G
6	a	1124	C
6	a	1125	C
6	a	1130	A
6	a	1138	U

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Mol	Chain	Res	Type
6	a	1139	G
6	a	1144	C
6	a	1148	A
6	a	1149	A
6	a	1150	G
6	a	1151	U
6	a	1152	U
6	a	1153	G
6	a	1157	A
6	a	1165	U
6	a	1168	A
6	a	1169	C
6	a	1179	C
6	a	1194	U
6	a	1195	G
6	a	1198	G
6	a	1202	A
6	a	1207	A
6	a	1208	A
6	a	1211	C
6	a	1223	U
6	a	1232	G
6	a	1238	A
6	a	1247	A
6	a	1248	C
6	a	1249	A
6	a	1250	A
6	a	1261	A
6	a	1268	A
6	a	1271	G
6	a	1279	G
6	a	1297	U
6	a	1298	A
6	a	1300	A
6	a	1304	G
6	a	1310	A
6	a	1311	G
6	a	1313	U
6	a	1328	C
6	a	1331	C
6	a	1333	C
6	a	1334	G

Continued on next page...

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Mol	Chain	Res	Type
6	a	1346	C
6	a	1347	U
6	a	1349	G
6	a	1351	A
6	a	1357	A
6	a	1375	U
6	a	1390	G
6	a	1392	U
6	a	1406	C
6	a	1409	A
6	a	1430	G
6	a	1436	A
6	a	1437	A
6	a	1451	U
6	a	1453	G
6	a	1457	A
6	a	1458	A
6	a	1459	C
6	a	1462	U
6	a	1463	U
6	a	1464	U
6	a	1465	A
6	a	1467	G
6	a	1504	A
6	a	1505	A
6	a	1509	G
6	a	1511	A
6	a	1515	A
6	a	1518	U
6	a	1519	A
6	a	1521	C
6	a	1529	G
6	a	1531	A
6	a	1541	G
6	a	1542	G
6	a	1546	A
6	a	1548	C
7	B	10	U
7	B	23	U
7	B	25	A
7	B	31	G
7	B	38	U

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Mol	Chain	Res	Type
7	B	40	C
7	B	42	G
7	B	54	U
7	B	55	A
7	B	83	C
7	B	85	U
7	B	87	C
7	B	88	G
7	B	100	U
7	B	106	G
7	B	109	G

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	22	A
5	A	298	U
5	A	475	A
5	A	517	A
5	A	640	G
5	A	756	A
5	A	1046	G
5	A	1310	A
5	A	1457	U
5	A	1651	C
5	A	1828	U
5	A	1874	A
5	A	1938	U
5	A	2135	U
5	A	2239	A
5	A	2432	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 162 ligands modelled in this entry, 160 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	ATP	0	603	54	32,33,33	0.65	1 (3%)	48,52,52	0.75	2 (4%)
55	ATP	0	604	54	32,33,33	0.52	0	48,52,52	0.71	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
55	ATP	0	603	54	-	5/22/38/38	0/3/3/3
55	ATP	0	604	54	-	8/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	0	603	ATP	PA-O3A	-2.24	1.57	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	0	603	ATP	O2'-C2'-C3'	-2.25	104.61	111.82
55	0	603	ATP	O3'-C3'-C2'	-2.04	105.29	111.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	0	603	ATP	C5'-O5'-PA-O1A
55	0	603	ATP	C5'-O5'-PA-O3A

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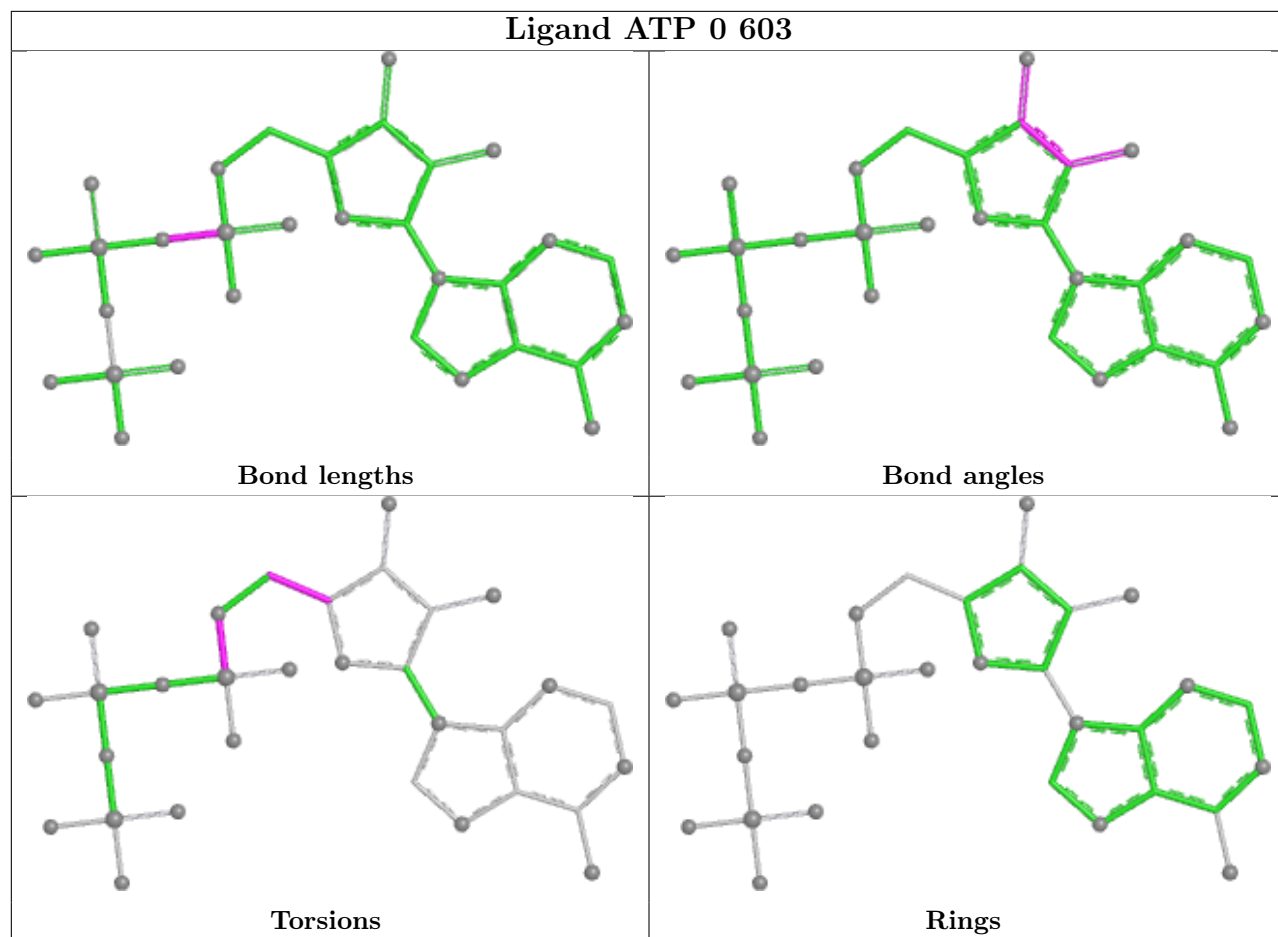
Mol	Chain	Res	Type	Atoms
55	0	604	ATP	PB-O3B-PG-O2G
55	0	604	ATP	C5'-O5'-PA-O3A
55	0	603	ATP	O4'-C4'-C5'-O5'
55	0	603	ATP	C3'-C4'-C5'-O5'
55	0	603	ATP	C5'-O5'-PA-O2A
55	0	604	ATP	C5'-O5'-PA-O1A
55	0	604	ATP	O4'-C4'-C5'-O5'
55	0	604	ATP	PG-O3B-PB-O1B
55	0	604	ATP	PG-O3B-PB-O2B
55	0	604	ATP	PA-O3A-PB-O2B
55	0	604	ATP	PB-O3B-PG-O1G

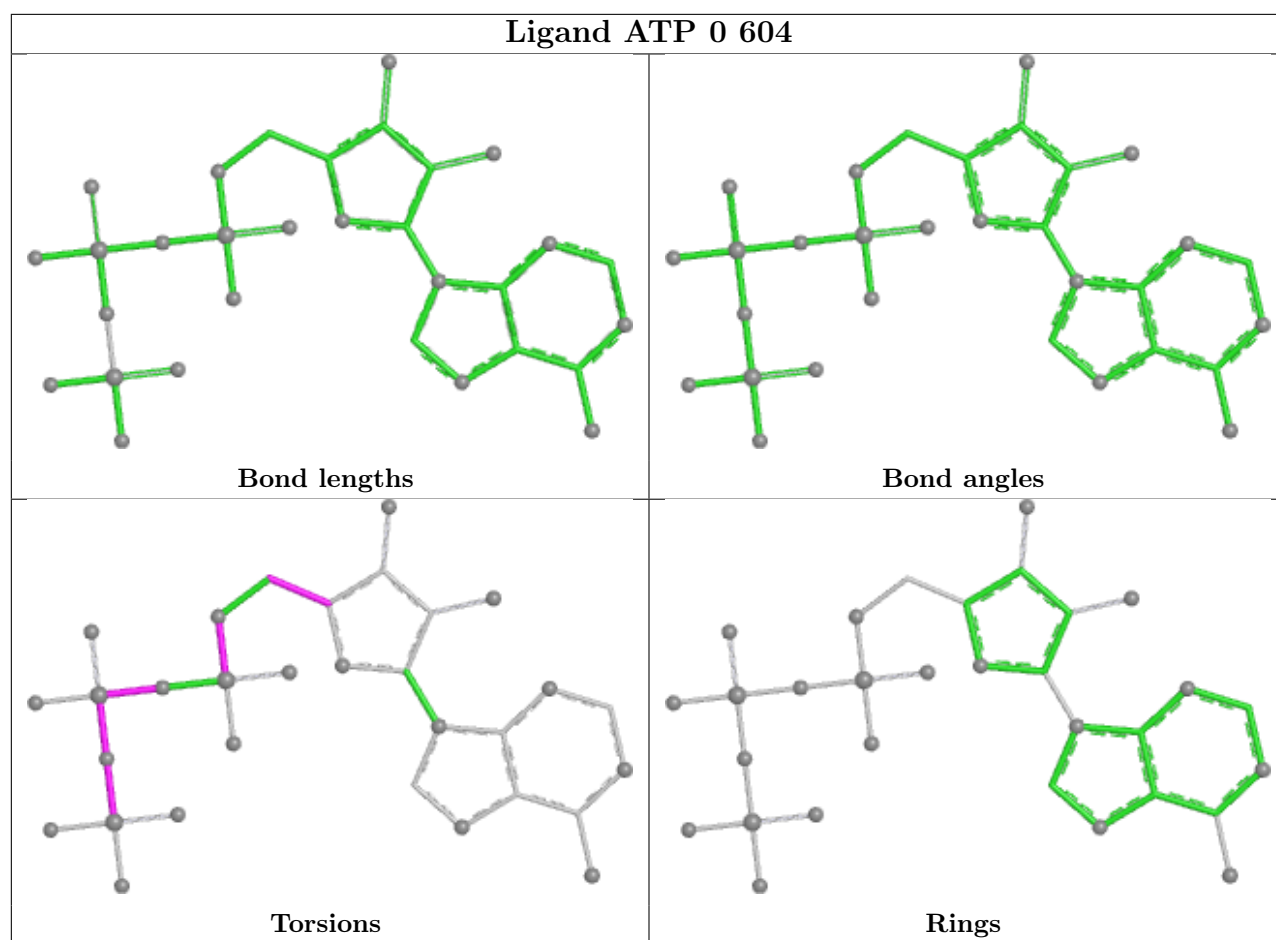
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	0	603	ATP	7	0
55	0	604	ATP	4	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

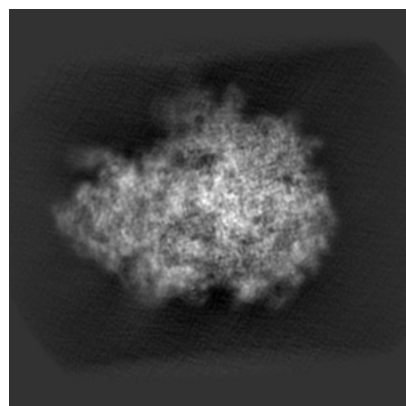
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12332. These allow visual inspection of the internal detail of the map and identification of artifacts.

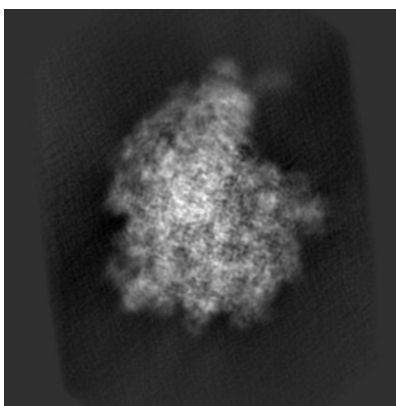
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

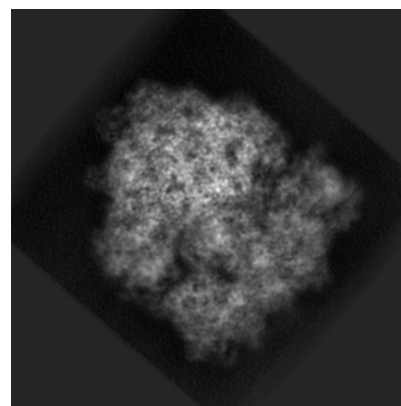
6.1.1 Primary map



X

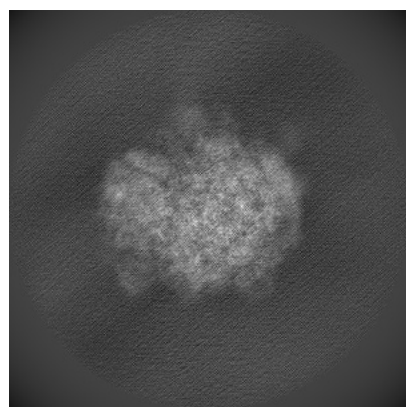


Y

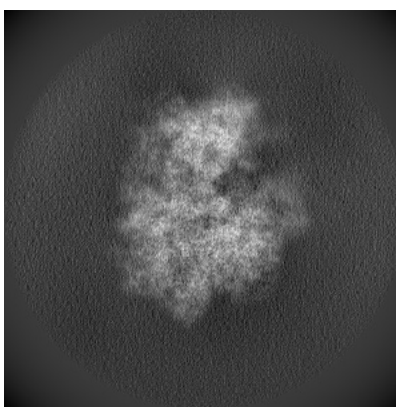


Z

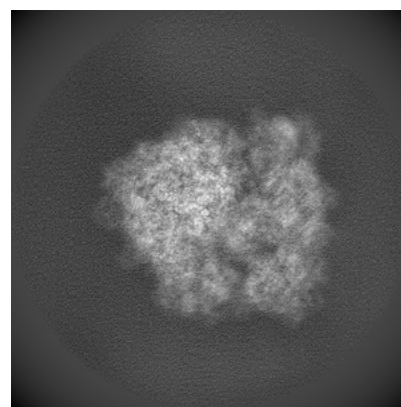
6.1.2 Raw map



X



Y

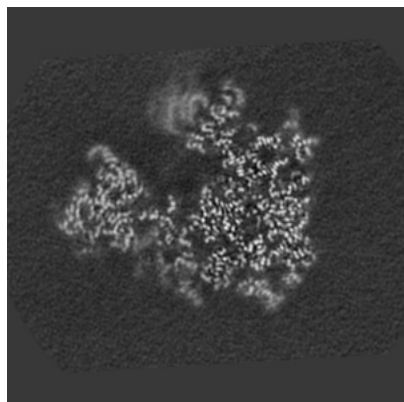


Z

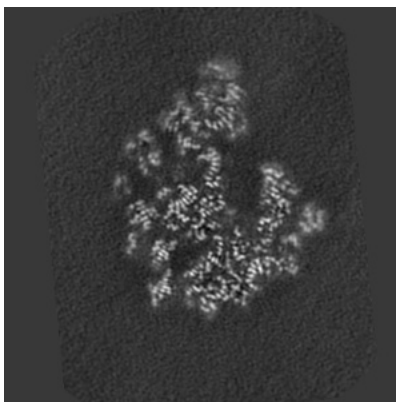
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

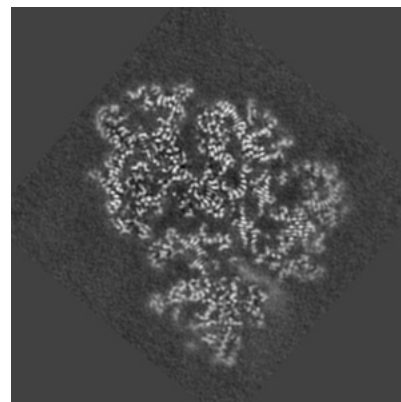
6.2.1 Primary map



X Index: 176

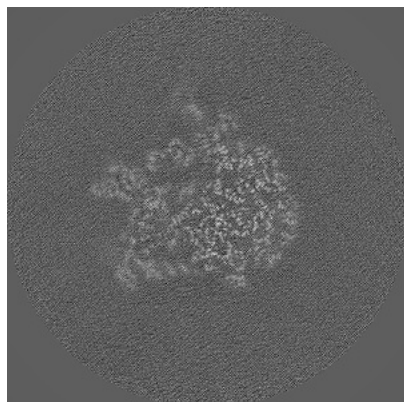


Y Index: 176

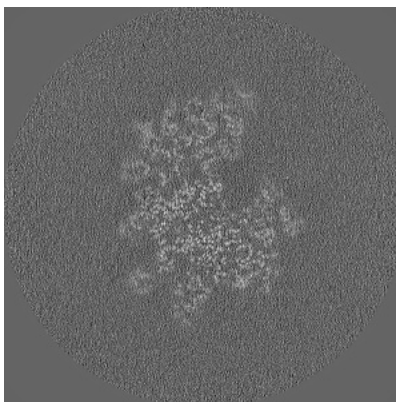


Z Index: 176

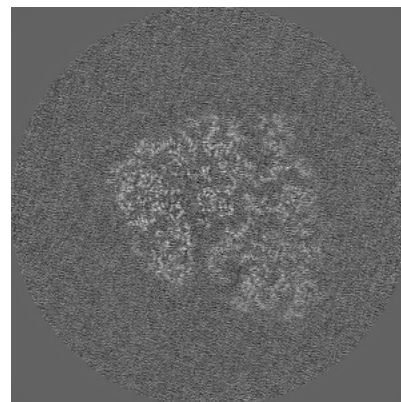
6.2.2 Raw map



X Index: 255



Y Index: 255

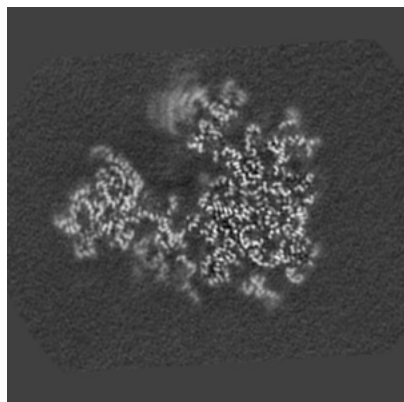


Z Index: 255

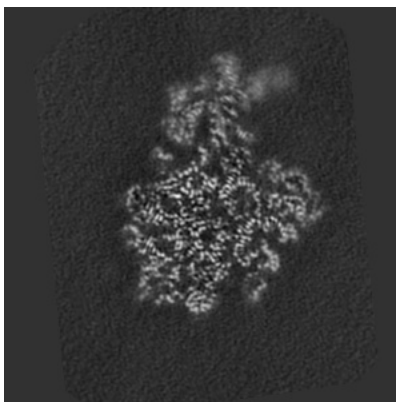
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

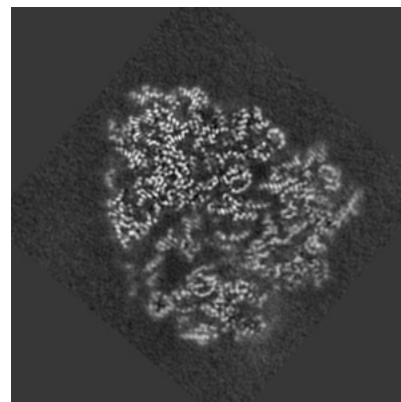
6.3.1 Primary map



X Index: 173

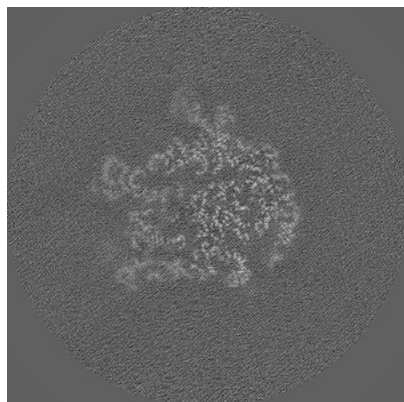


Y Index: 189

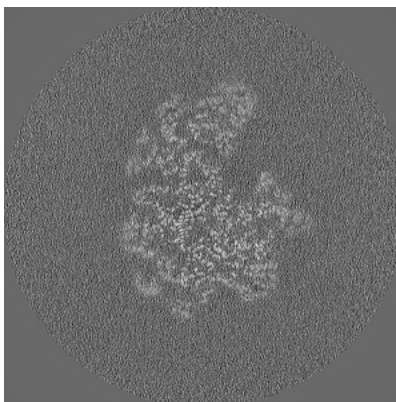


Z Index: 186

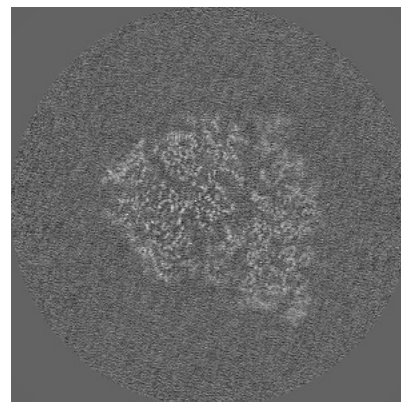
6.3.2 Raw map



X Index: 249



Y Index: 268

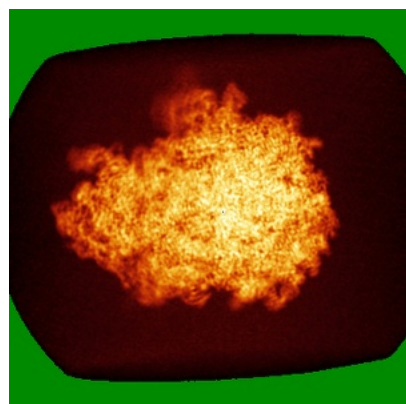


Z Index: 249

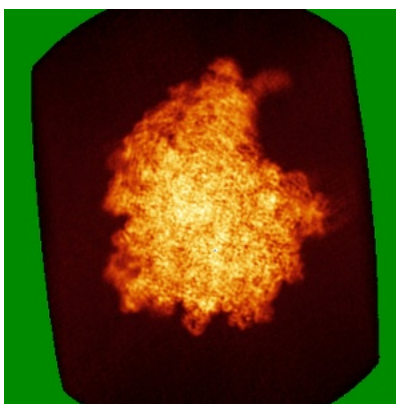
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

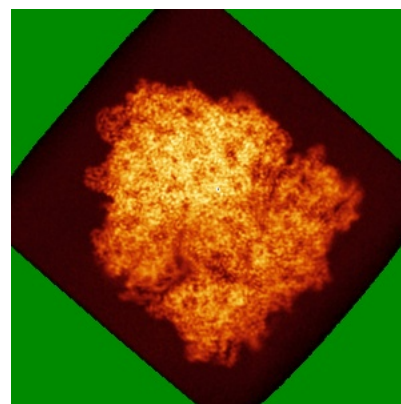
6.4.1 Primary map



X

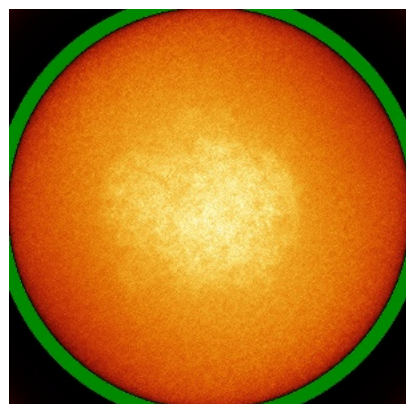


Y

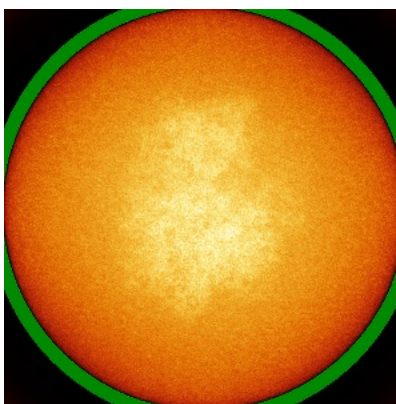


Z

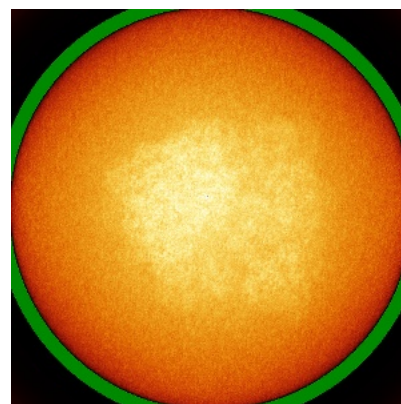
6.4.2 Raw map



X



Y

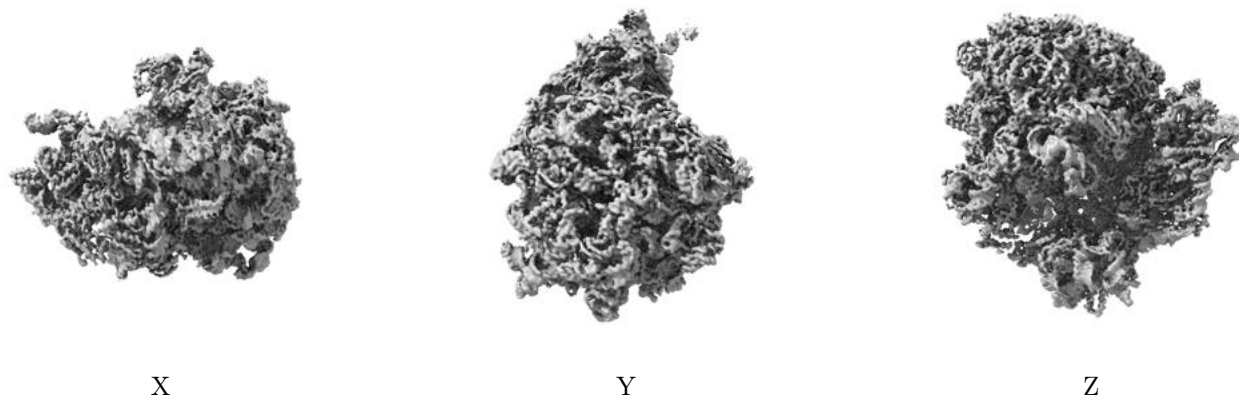


Z

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.

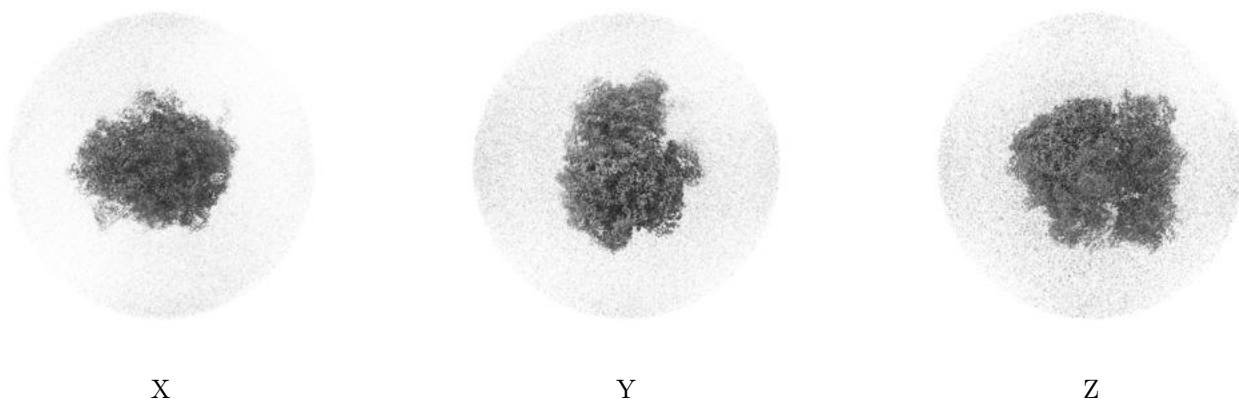
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

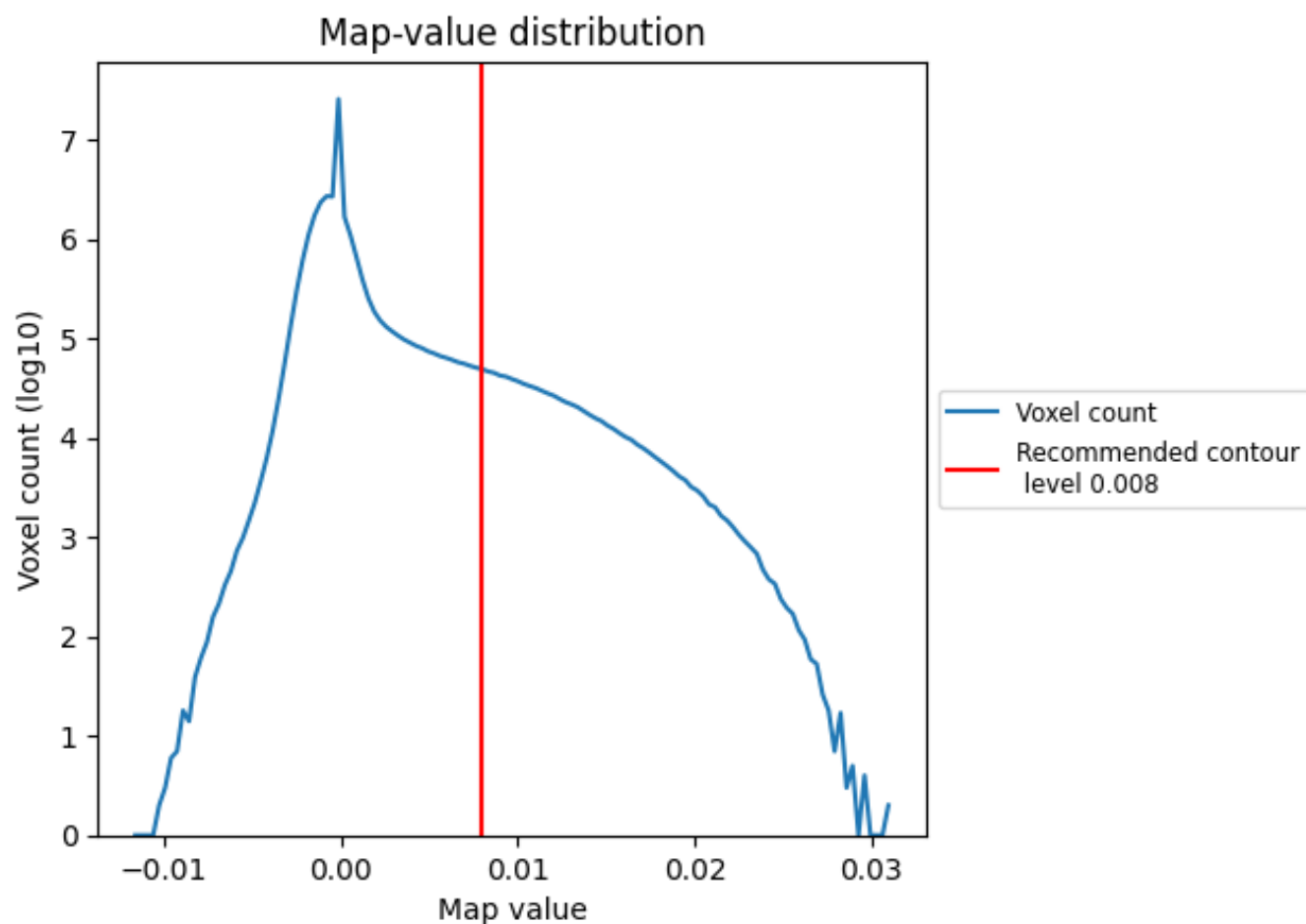
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

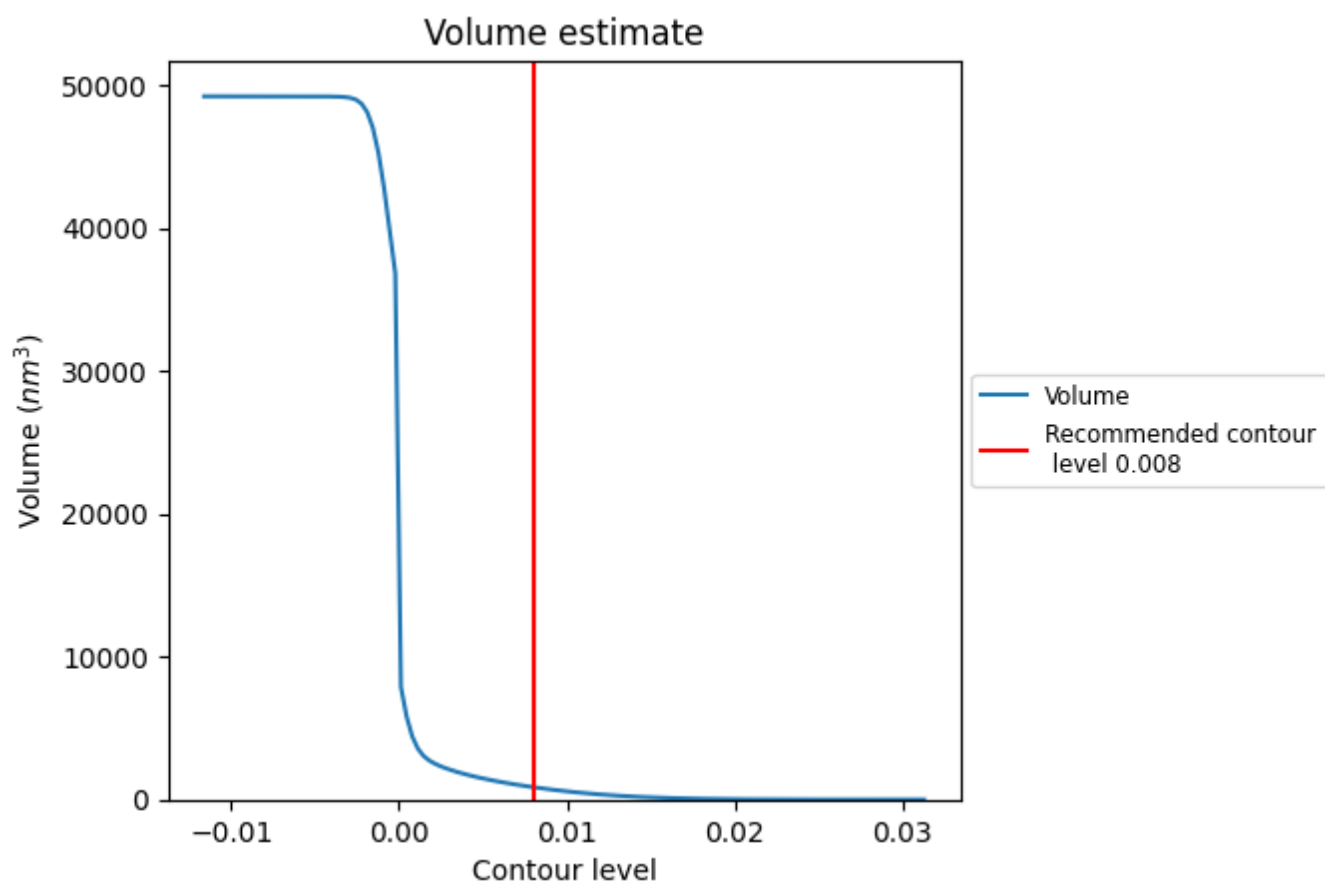
This section contains the results of statistical analysis of the map.

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.

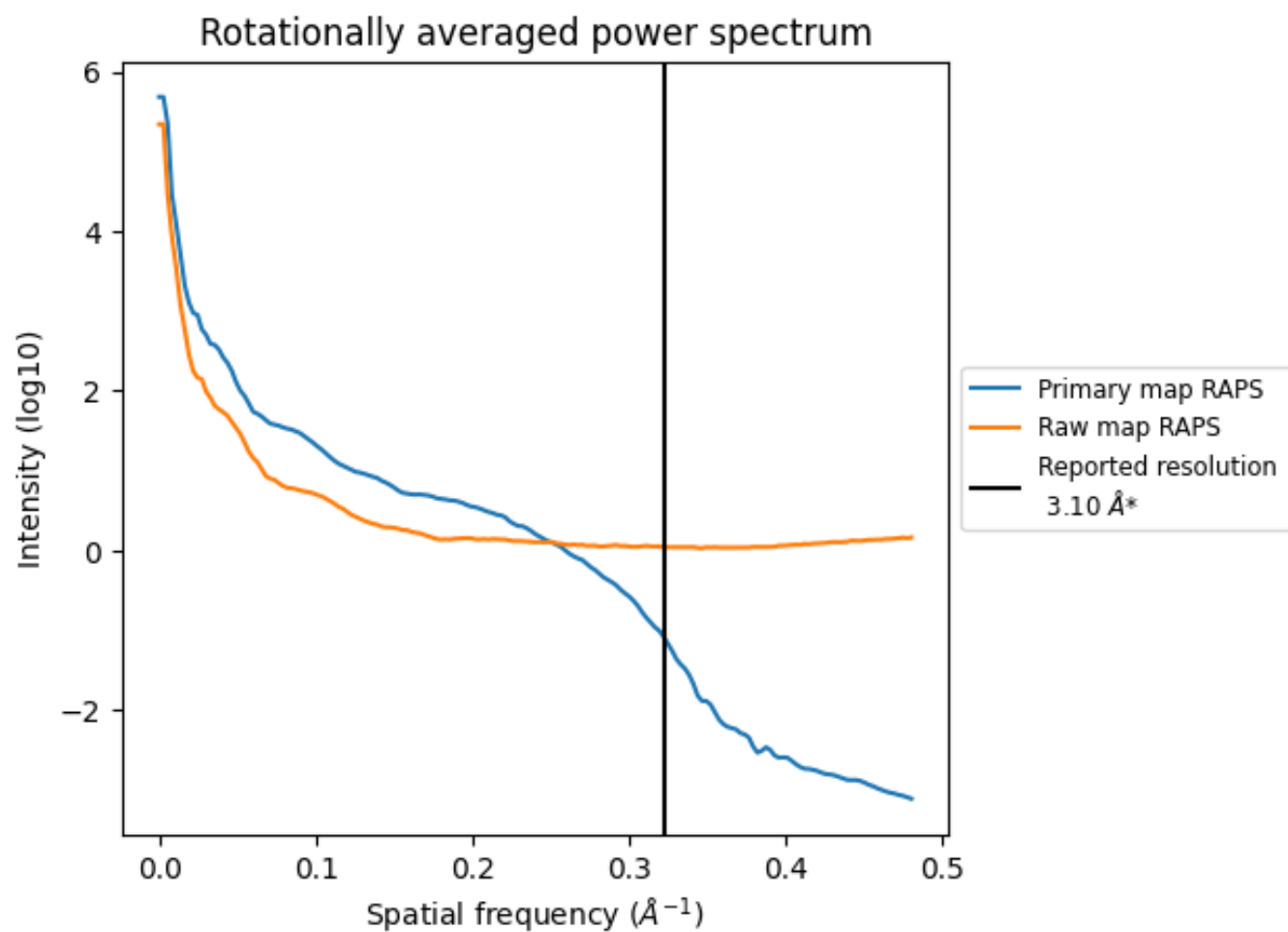
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 865 nm^3 ; this corresponds to an approximate mass of 782 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 ⓘ

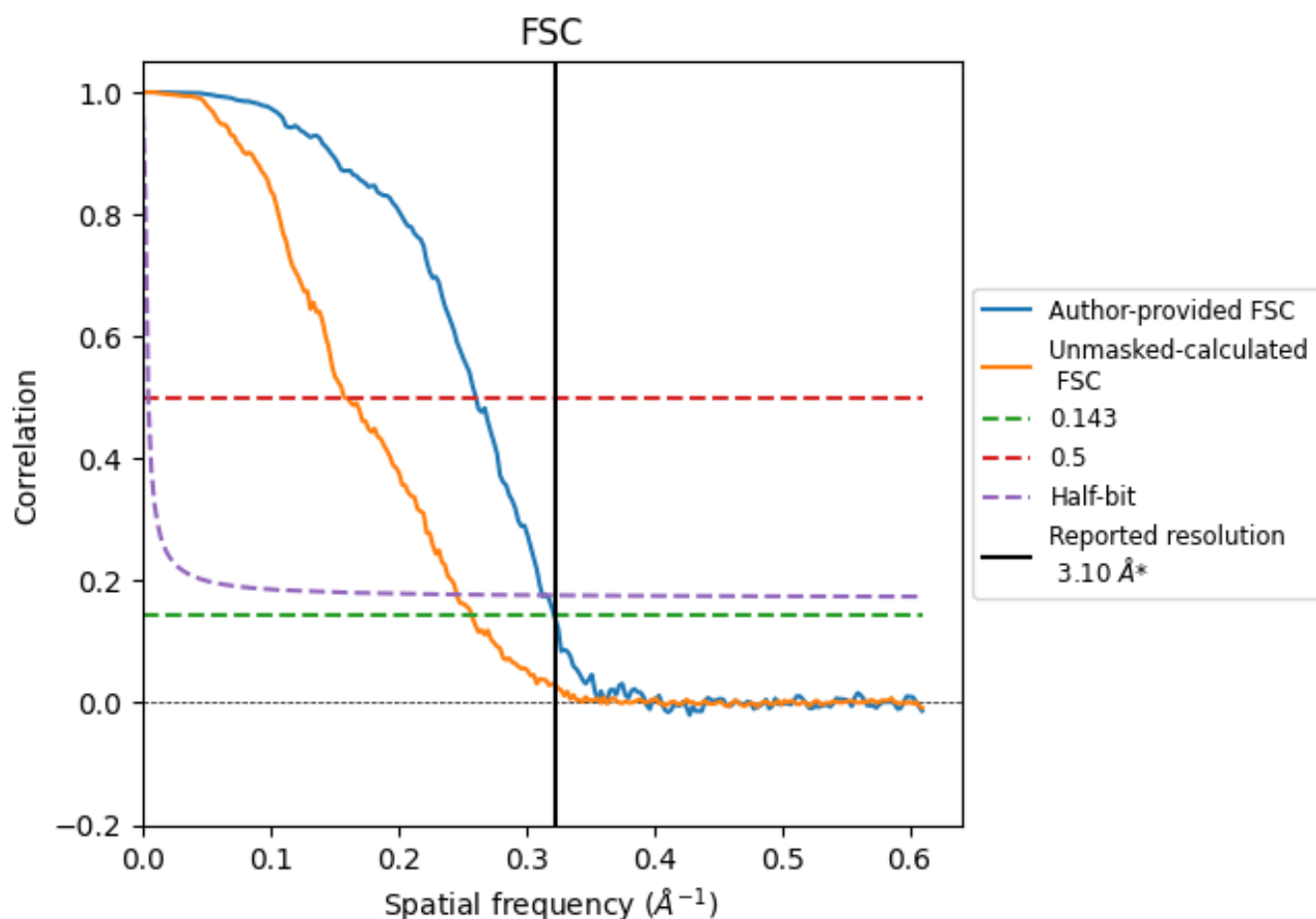


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

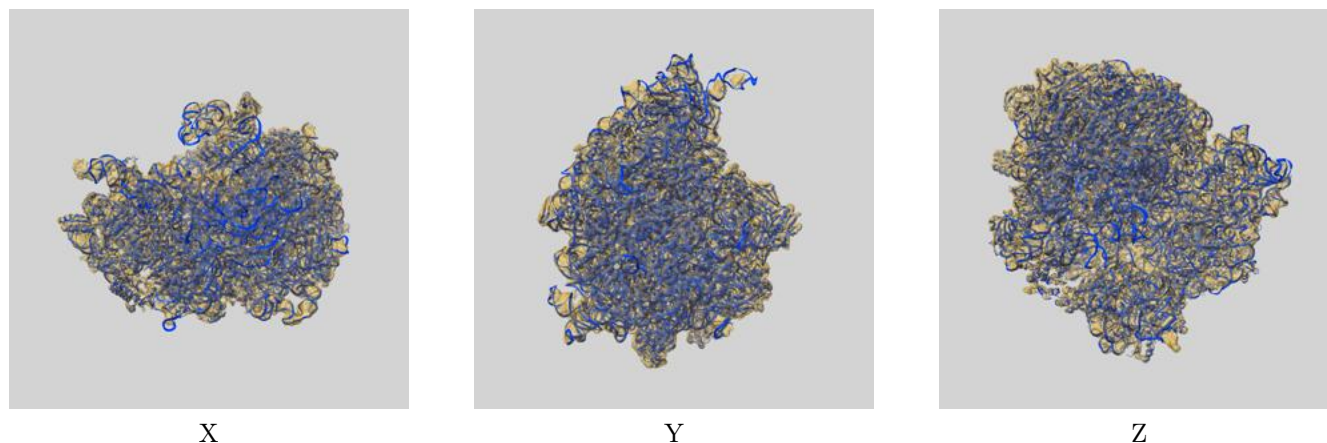
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.83	3.20
Unmasked-calculated*	3.88	6.34	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

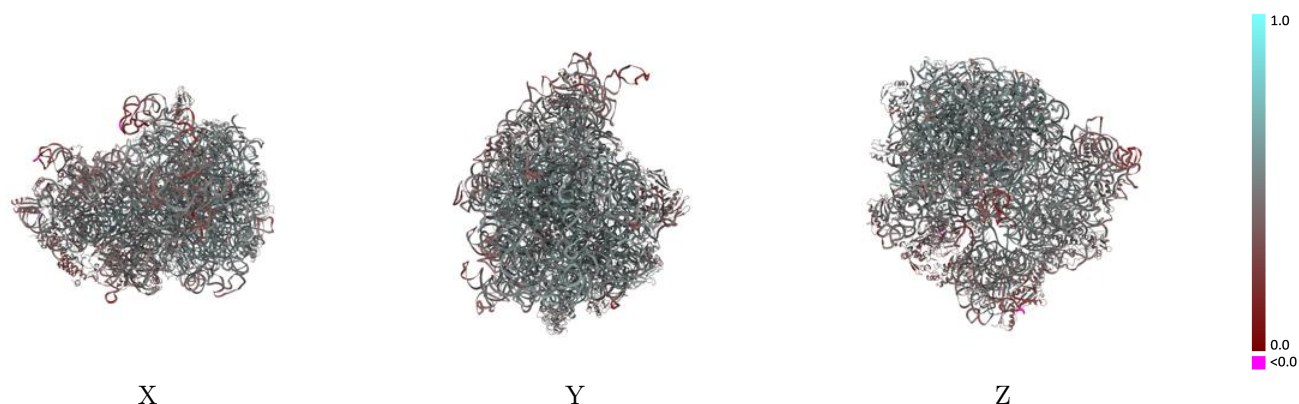
This section contains information regarding the fit between EMDB map EMD-12332 and PDB model 7NHL. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



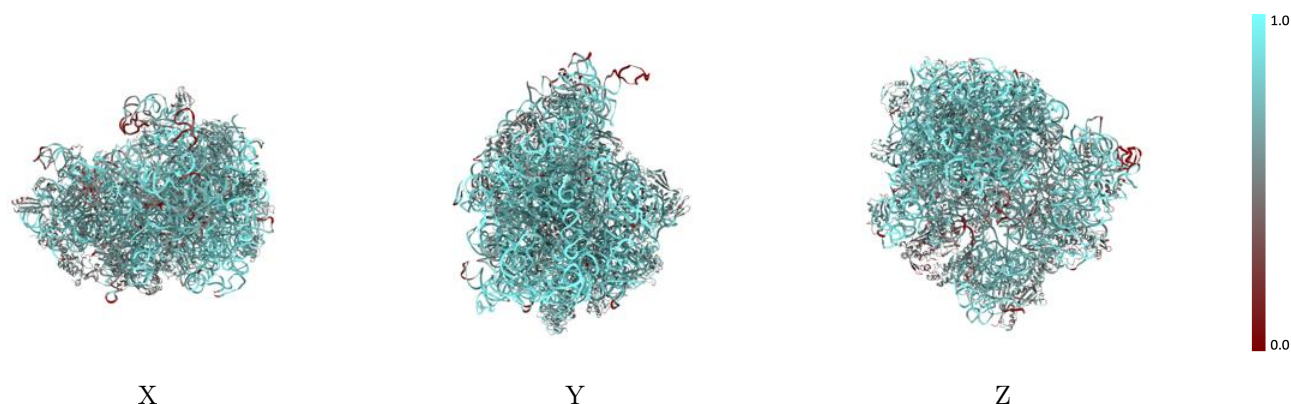
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



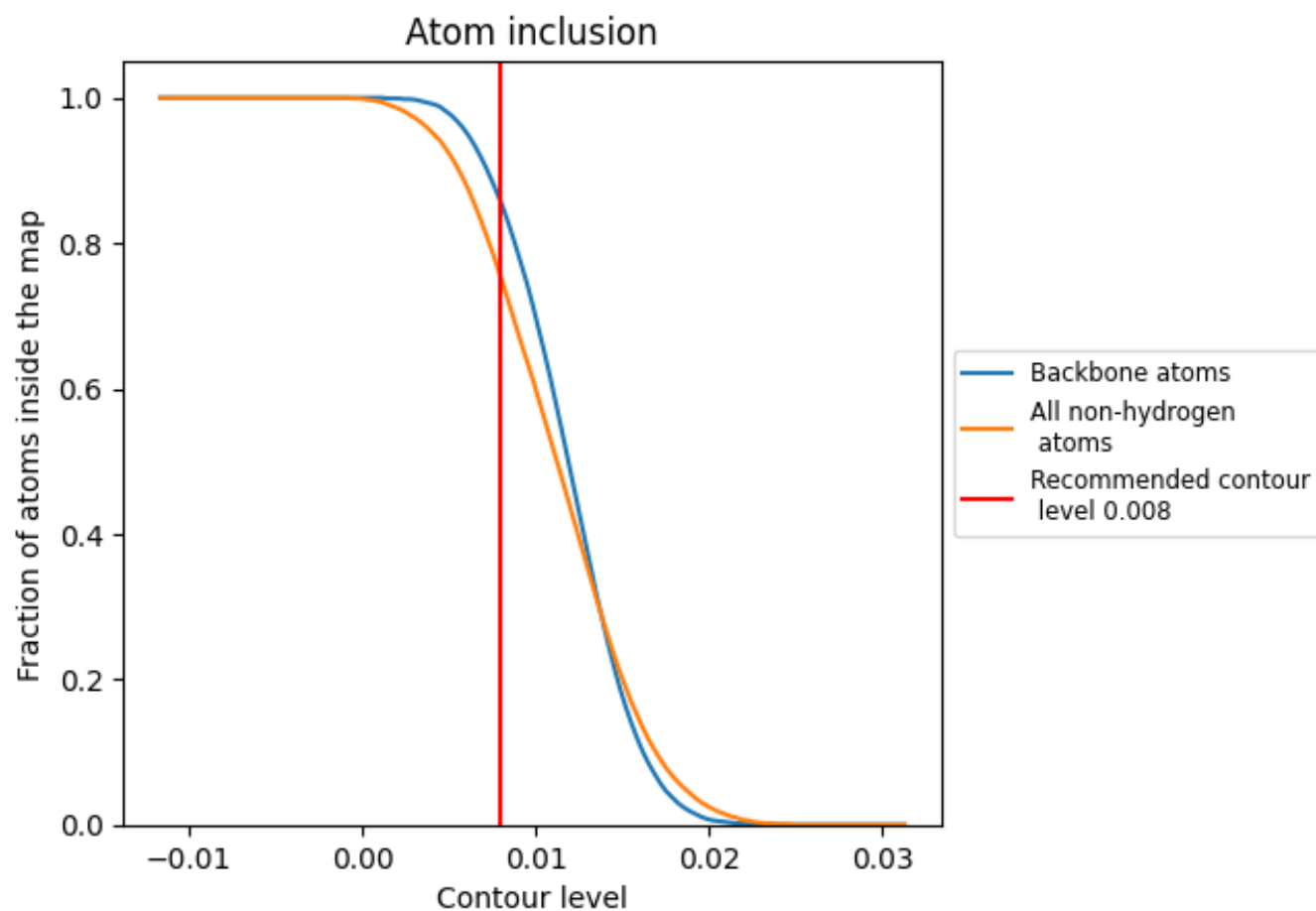
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7530	 0.4760
0	 0.4910	 0.4250
1	 0.5720	 0.4960
2	 0.6480	 0.4410
3	 0.6350	 0.4720
4	 0.3360	 0.3180
5	 0.6920	 0.5010
6	 0.6680	 0.4730
7	 0.7080	 0.5400
8	 0.6690	 0.5280
9	 0.6720	 0.5070
A	 0.8530	 0.5040
B	 0.8400	 0.4520
D	 0.7730	 0.4950
G	 0.6530	 0.5140
H	 0.6600	 0.5050
I	 0.6530	 0.4850
J	 0.4500	 0.3630
K	 0.5590	 0.4100
M	 0.6580	 0.4900
N	 0.5690	 0.5020
O	 0.6550	 0.5010
P	 0.6330	 0.4980
Q	 0.6570	 0.4820
R	 0.5860	 0.4210
S	 0.5900	 0.4790
T	 0.6860	 0.4860
U	 0.6540	 0.4980
V	 0.6640	 0.5110
W	 0.6380	 0.4950
X	 0.5800	 0.4610
Y	 0.5520	 0.4350
Z	 0.6520	 0.5060
a	 0.8090	 0.4640
b	 0.6480	 0.4650



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Chain	Atom inclusion	Q-score
c	 0.4800	 0.3840
d	 0.5820	 0.4200
e	 0.4530	 0.4120
f	 0.5940	 0.4640
g	 0.4340	 0.3820
h	 0.6230	 0.4040
i	 0.5150	 0.4280
j	 0.6290	 0.4420
k	 0.5310	 0.4020
l	 0.4120	 0.3920
m	 0.5010	 0.4560
n	 0.5100	 0.3990
o	 0.6240	 0.4510
p	 0.5210	 0.3910
q	 0.4730	 0.4030
r	 0.4700	 0.4350
s	 0.4900	 0.4130
t	 0.4690	 0.4020
u	 0.5050	 0.3850