



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:36 AM UTC

PDB ID : 8B7Y / pdb_00008b7y
EMDB ID : EMD-15905
Title : Cryo-EM structure of the E.coli 70S ribosome in complex with the antibiotic Myxovalargin B.
Authors : Koller, T.O.; Graf, M.; Wilson, D.N.
Deposited on : 2022-10-03
Resolution : 3.00 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:

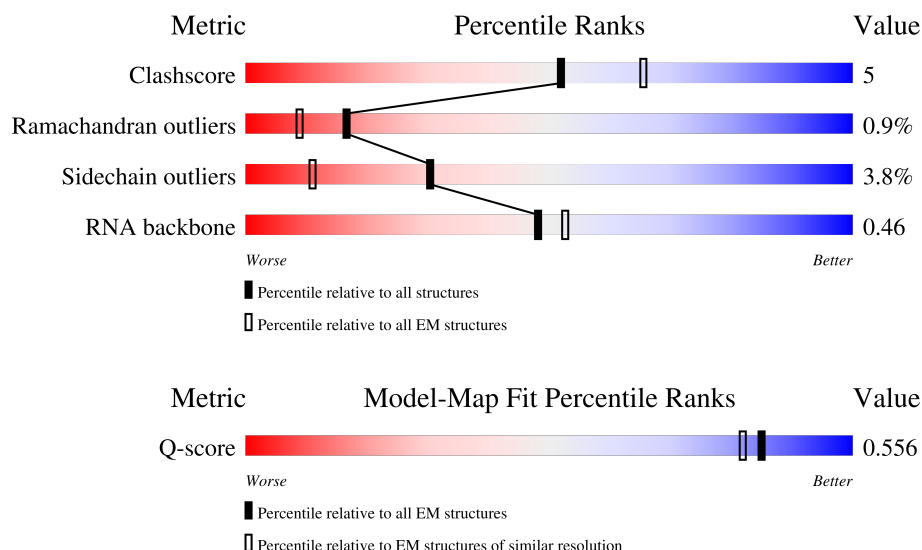
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.00 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	14081 (2.50 - 3.50)

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	I	2904	
2	J	118	
3	K	273	

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Mol	Chain	Length	Quality of chain
4	L	209	
5	M	201	
6	O	177	
7	R	142	
8	S	123	
9	T	144	
10	U	136	
11	V	127	
12	W	117	
13	X	115	
14	Y	118	
15	Z	103	
16	a	110	
17	b	100	
18	c	104	
19	d	94	
20	e	85	
21	f	78	
22	g	63	
23	h	59	
24	i	57	
25	j	55	
26	k	46	
27	l	65	
28	m	38	

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Mol	Chain	Length	Quality of chain
29	n	76	
30	C	1533	
31	D	241	
32	E	233	
33	F	206	
34	G	167	
35	H	135	
36	N	179	
37	P	130	
38	Q	130	
39	o	103	
40	p	129	
41	q	124	
42	r	118	
43	s	101	
44	t	89	
45	u	82	
46	v	84	
47	w	75	
48	x	92	
49	y	87	
50	5	71	
51	6	3	
52	z	16	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	FME	n	101	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 141008 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	2898	Total	C	N	O	P	0	0
			62225	27764	11448	20115	2898		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L6.

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

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

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

- Molecule 10 is a protein called 50S ribosomal protein L16.

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

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 12 is a protein called 50S ribosomal protein L18.

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

- Molecule 13 is a protein called 50S ribosomal protein L19.

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

- Molecule 14 is a protein called 50S ribosomal protein L20.

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

- Molecule 15 is a protein called 50S ribosomal protein L21.

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

- Molecule 16 is a protein called 50S ribosomal protein L22.

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

- Molecule 17 is a protein called 50S ribosomal protein L23.

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

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	102	Total	C	N	O		0
			779	492	146	141		0

- Molecule 19 is a protein called 50S ribosomal protein L25.

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

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	e	75	Total	C	N	O	S	0
			569	353	113	102	1	0

- Molecule 21 is a protein called 50S ribosomal protein L28.

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

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

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L32.

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

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	j	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 26 is a protein called 50S ribosomal protein L34.

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

- Molecule 27 is a protein called 50S ribosomal protein L35.

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

- Molecule 28 is a protein called 50S ribosomal protein L36.

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

- Molecule 29 is a RNA chain called P-tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	n	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C	1519	Total	C	N	O	P	0	0
			32599	14539	5986	10555	1519		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	5	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 51 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	6	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 52 is a protein (with D amino acids) called Myxovalargin B.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	z	16	Total	C	N	O	0	0
			118	80	21	17		

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	I	136	Total	Mg	0
			136	136	
53	J	2	Total	Mg	0
			2	2	
53	K	1	Total	Mg	0
			1	1	
53	T	1	Total	Mg	0
			1	1	
53	V	1	Total	Mg	0
			1	1	
53	a	2	Total	Mg	0
			2	2	
53	d	1	Total	Mg	0
			1	1	
53	h	1	Total	Mg	0
			1	1	
53	C	87	Total	Mg	0
			87	87	

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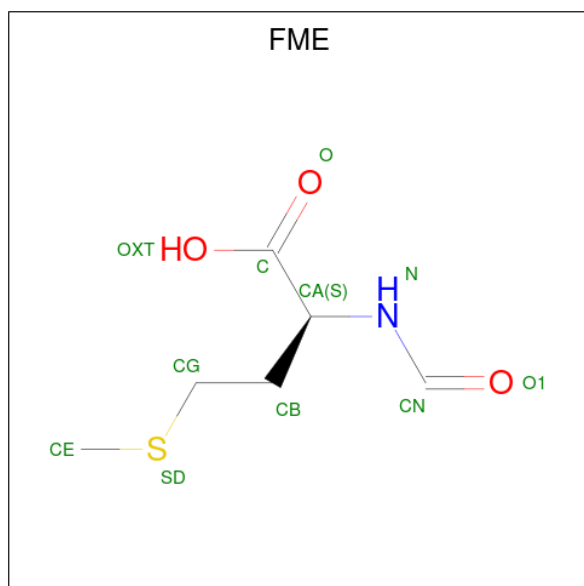
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Mol	Chain	Residues	Atoms		AltConf
53	G	1	Total	Mg	0
			1	1	
53	q	1	Total	Mg	0
			1	1	
53	s	1	Total	Mg	0
			1	1	
53	5	1	Total	Mg	0
			1	1	
53	6	1	Total	Mg	0
			1	1	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

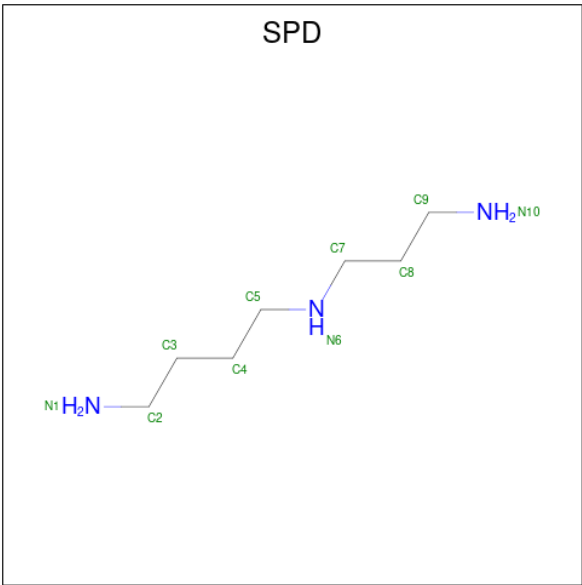
Mol	Chain	Residues	Atoms		AltConf
54	m	1	Total	Zn	0
			1	1	

- Molecule 55 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
55	n	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 56 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



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

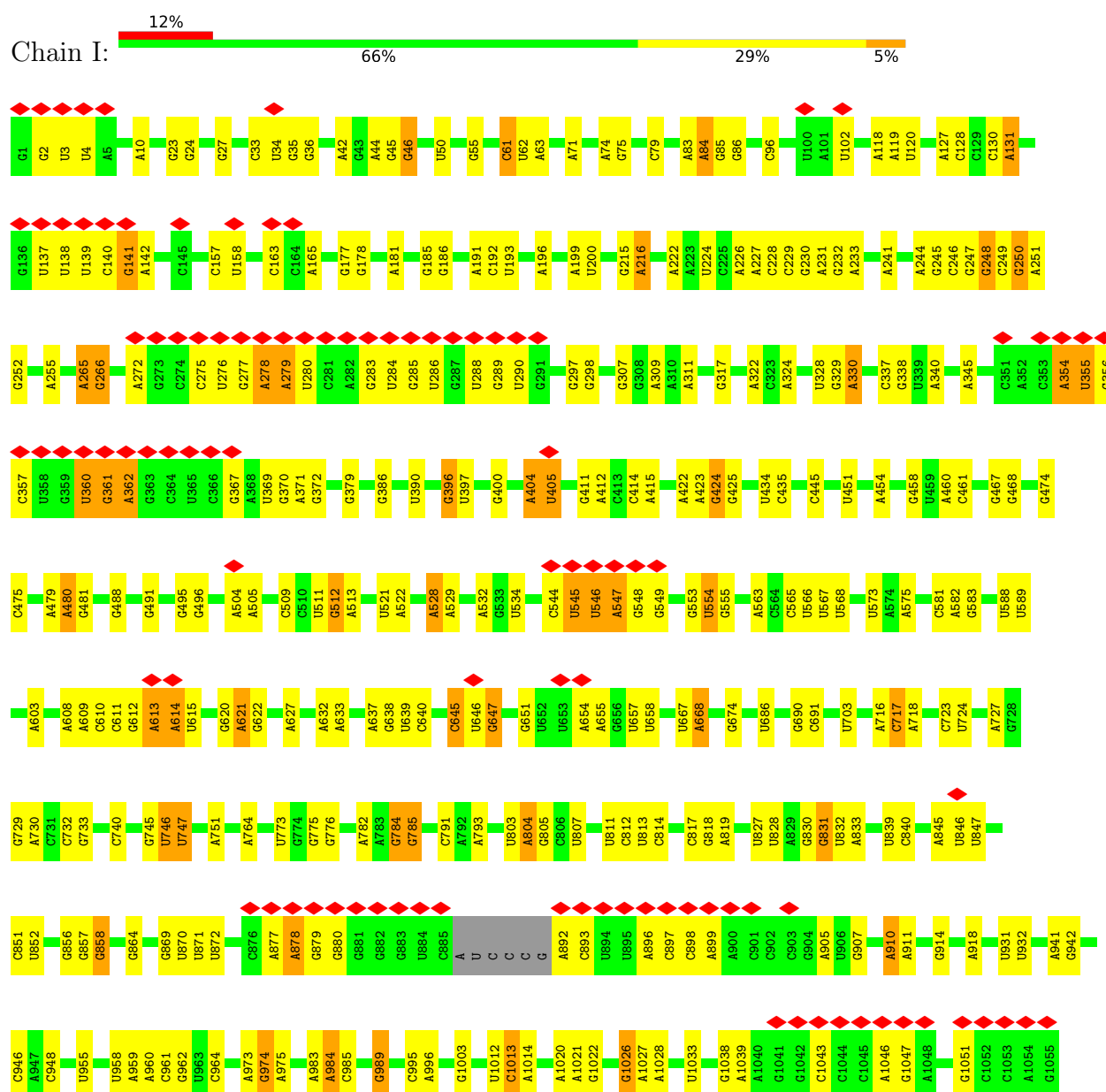
- Molecule 57 is water.

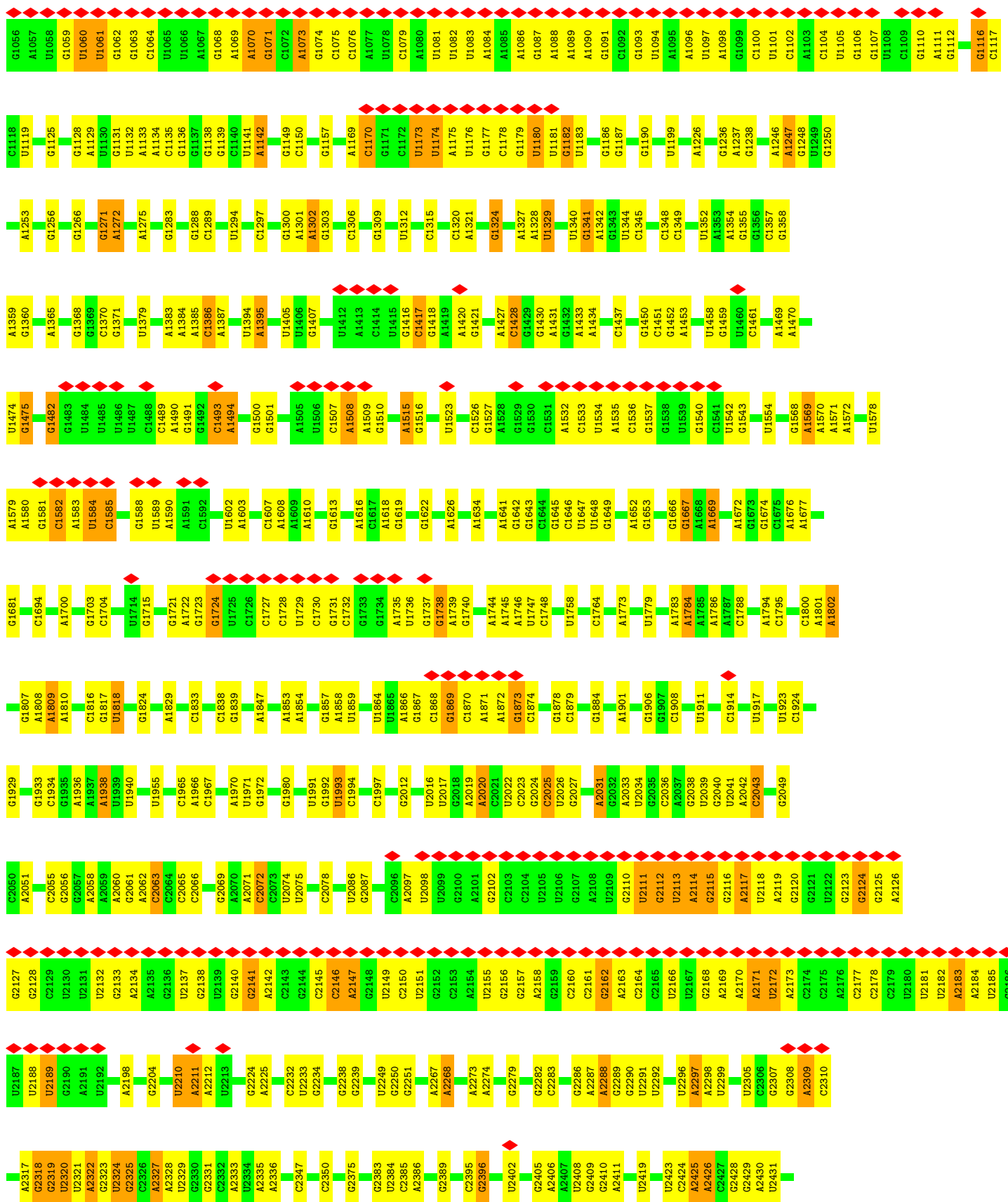
Mol	Chain	Residues	Atoms		AltConf
57	I	18	Total	O	0
			18	18	
57	z	10	Total	O	0
			10	10	

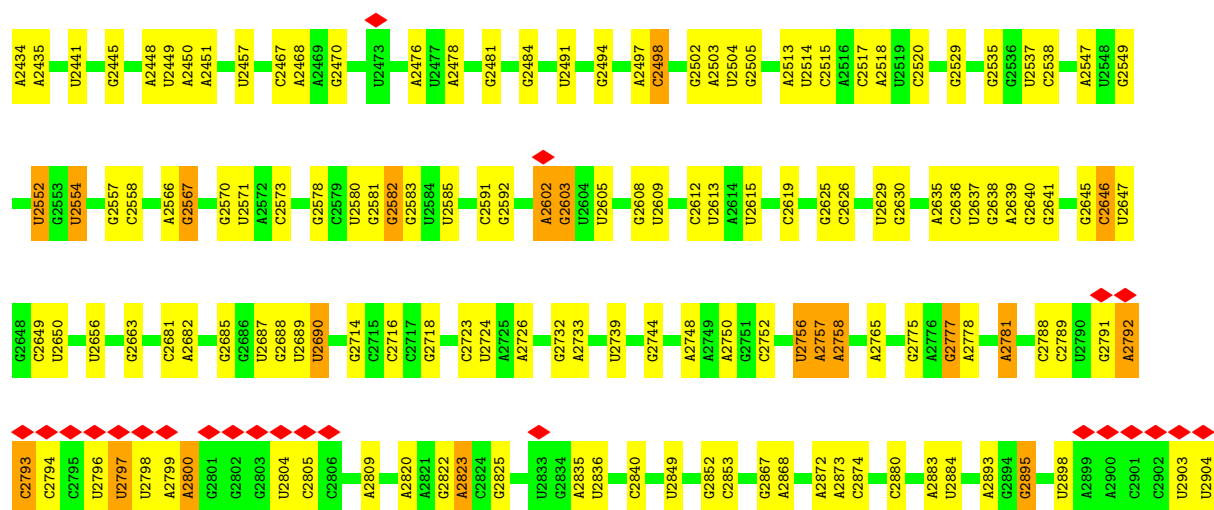
3 Residue-property plots

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.

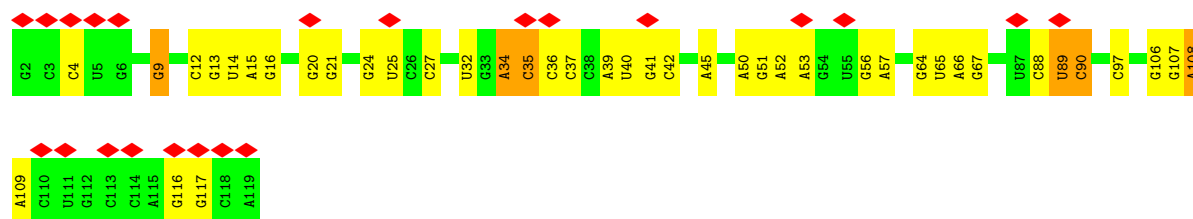
• Molecule 1: 23S ribosomal RNA



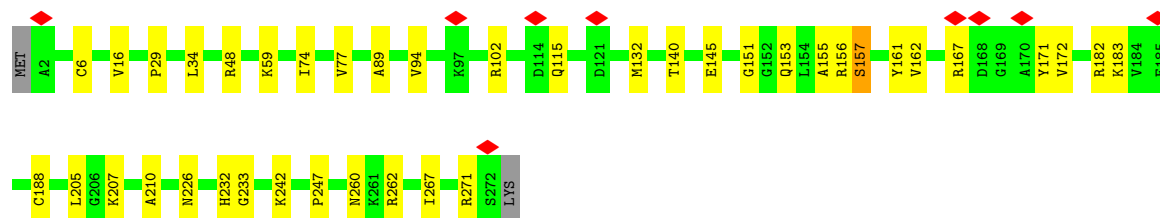
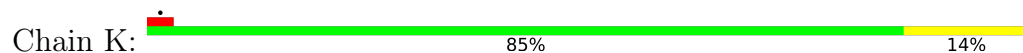




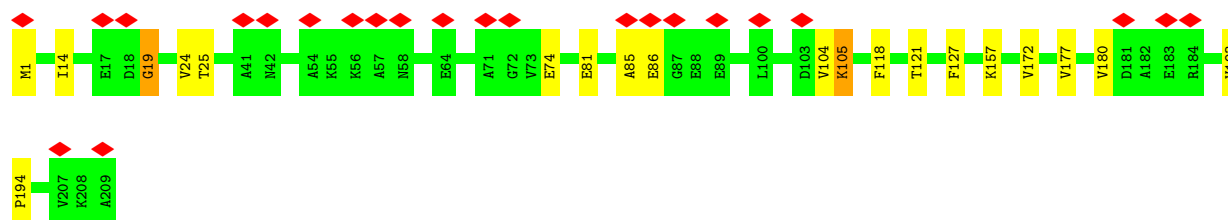
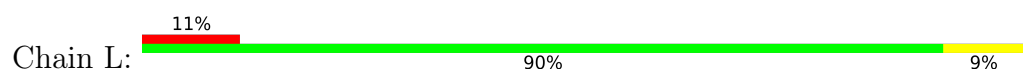
• Molecule 2: 5S ribosomal RNA



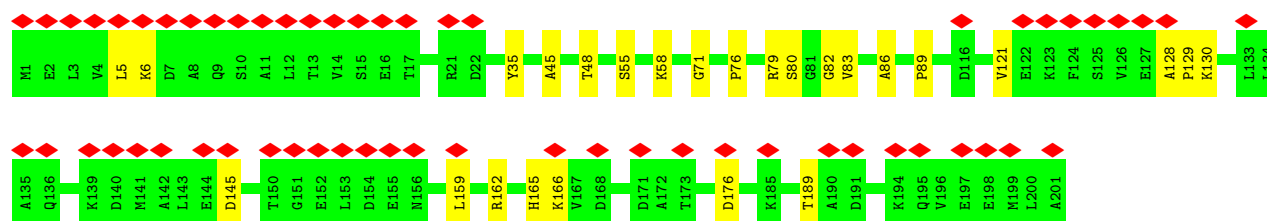
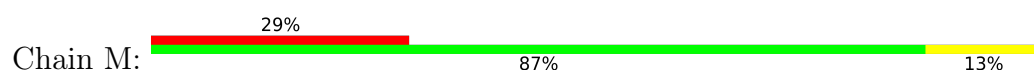
• Molecule 3: 50S ribosomal protein L2



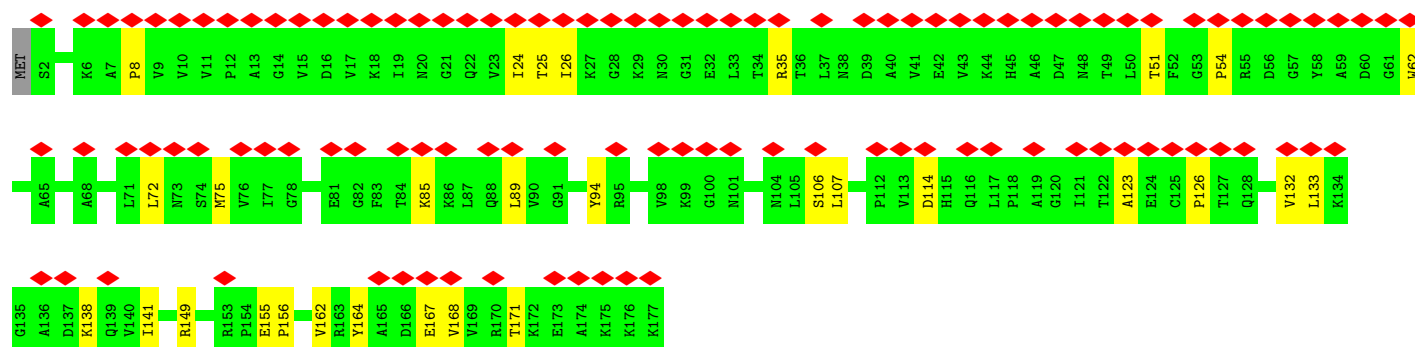
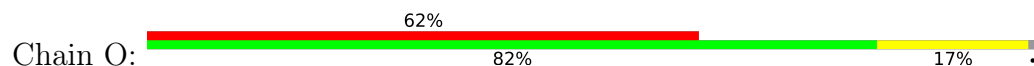
• Molecule 4: 50S ribosomal protein L3



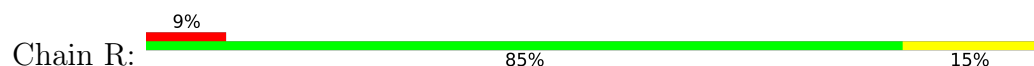
• Molecule 5: 50S ribosomal protein L4



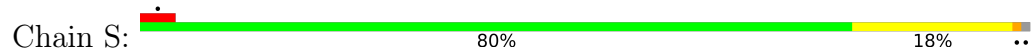
• Molecule 6: 50S ribosomal protein L6



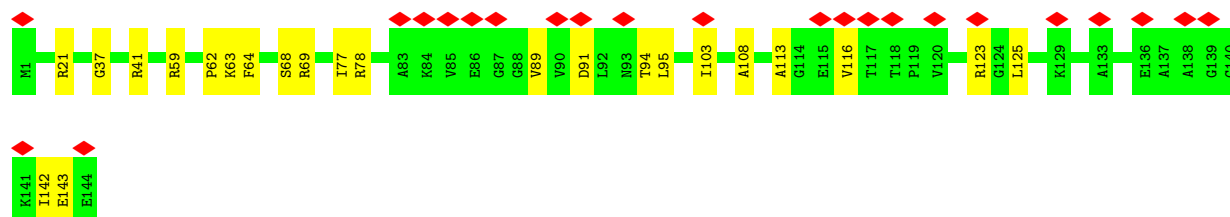
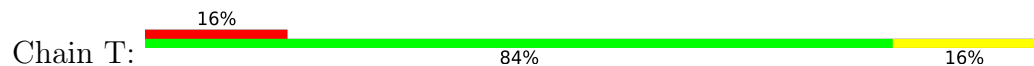
• Molecule 7: 50S ribosomal protein L13



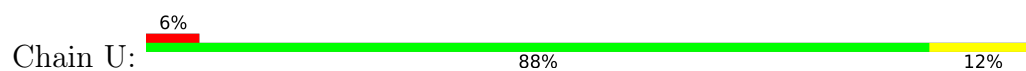
• Molecule 8: 50S ribosomal protein L14



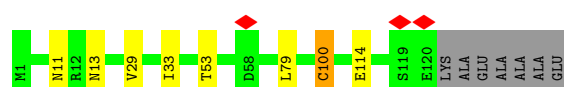
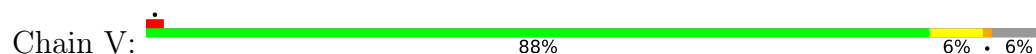
• Molecule 9: 50S ribosomal protein L15



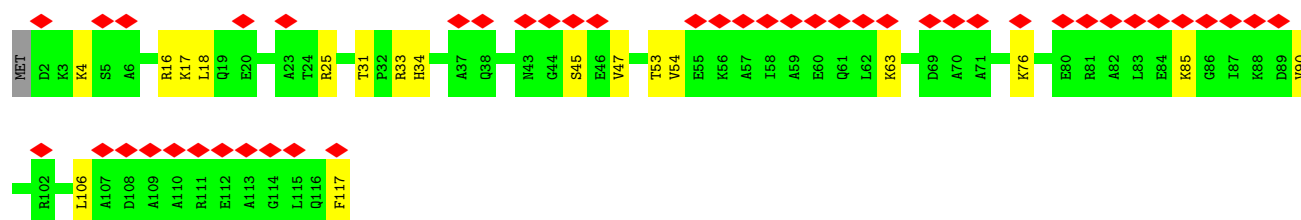
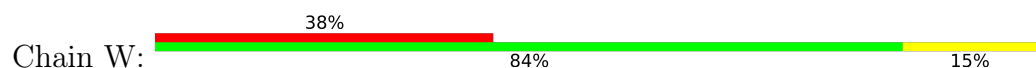
- Molecule 10: 50S ribosomal protein L16



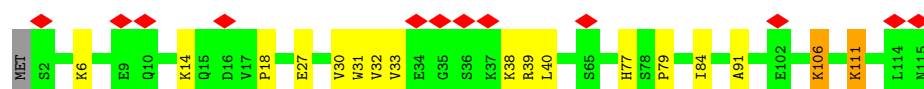
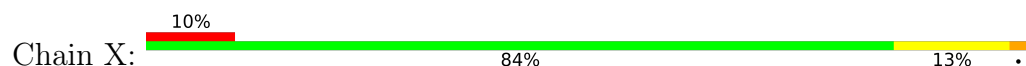
- Molecule 11: 50S ribosomal protein L17



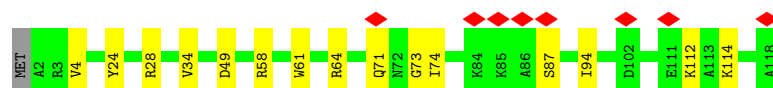
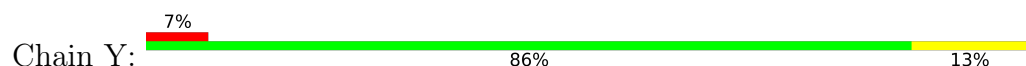
- Molecule 12: 50S ribosomal protein L18



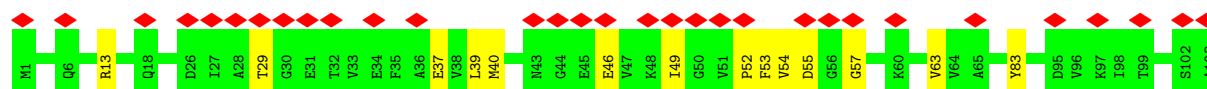
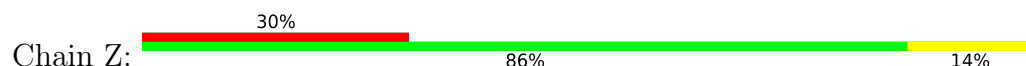
- Molecule 13: 50S ribosomal protein L19



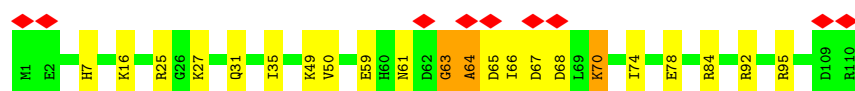
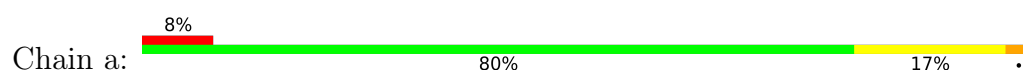
- Molecule 14: 50S ribosomal protein L20



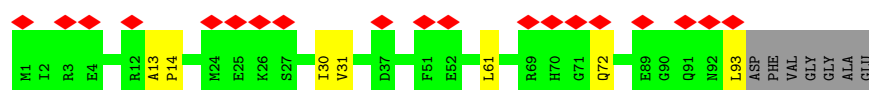
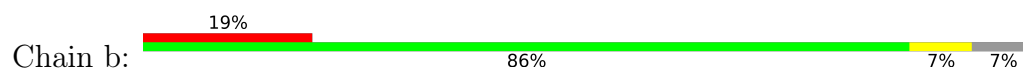
- Molecule 15: 50S ribosomal protein L21



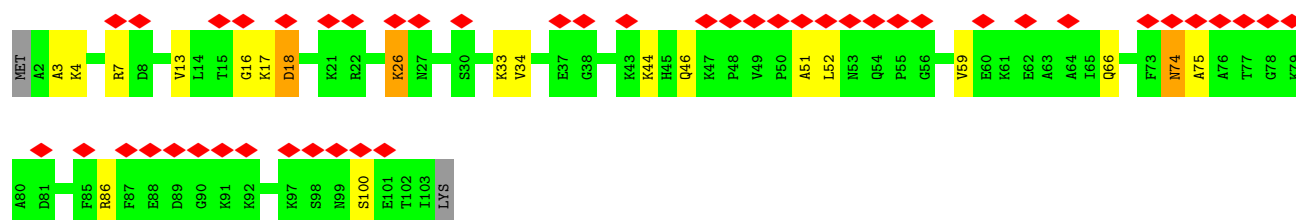
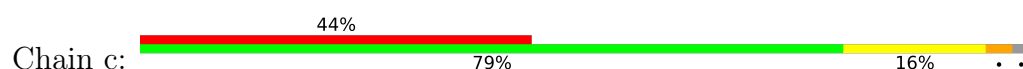
- Molecule 16: 50S ribosomal protein L22



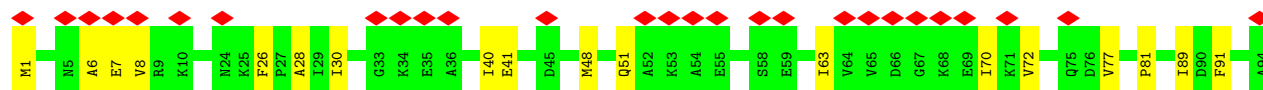
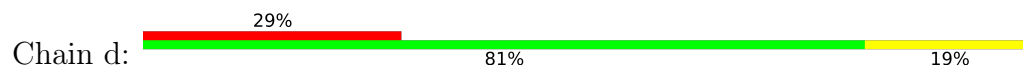
- Molecule 17: 50S ribosomal protein L23



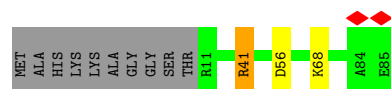
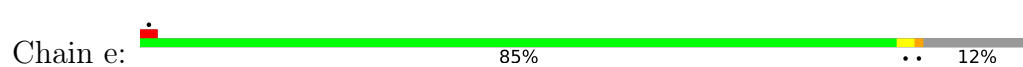
- Molecule 18: 50S ribosomal protein L24



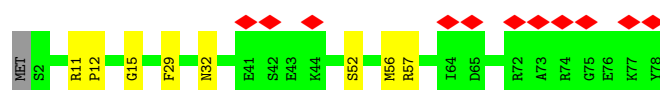
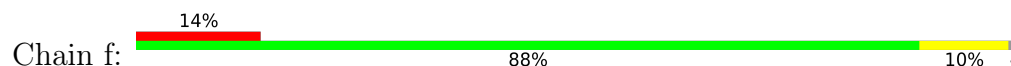
- Molecule 19: 50S ribosomal protein L25



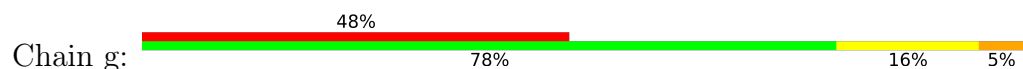
- Molecule 20: 50S ribosomal protein L27

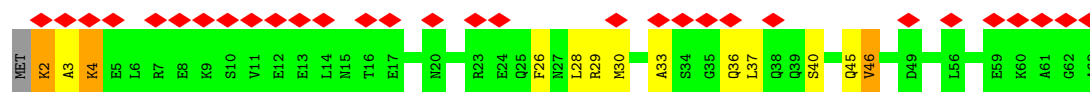


- Molecule 21: 50S ribosomal protein L28

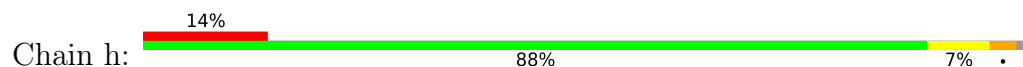


- Molecule 22: 50S ribosomal protein L29





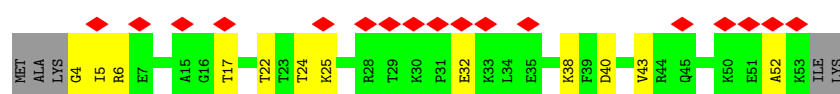
- Molecule 23: 50S ribosomal protein L30



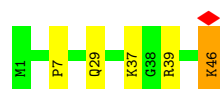
- Molecule 24: 50S ribosomal protein L32



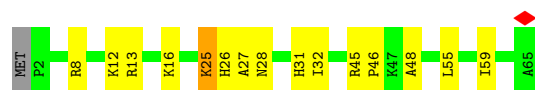
- Molecule 25: 50S ribosomal protein L33



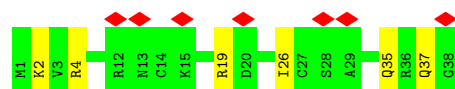
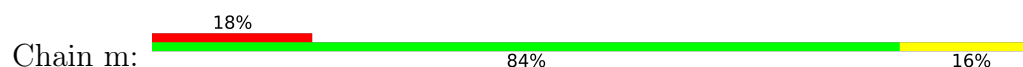
- Molecule 26: 50S ribosomal protein L34



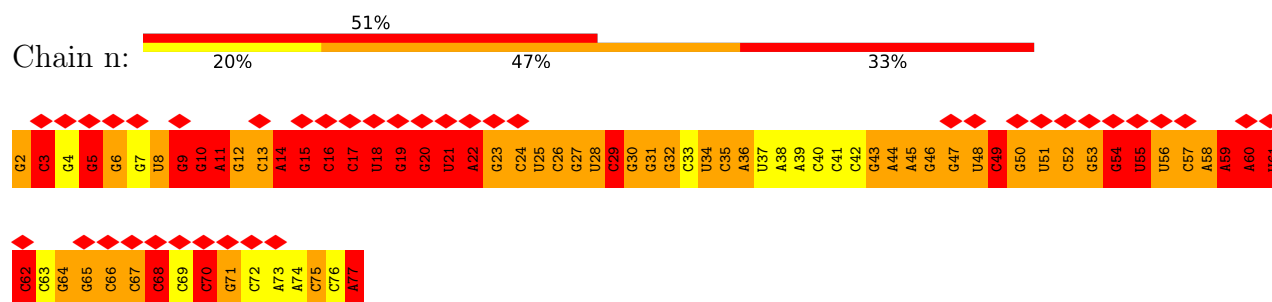
- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36

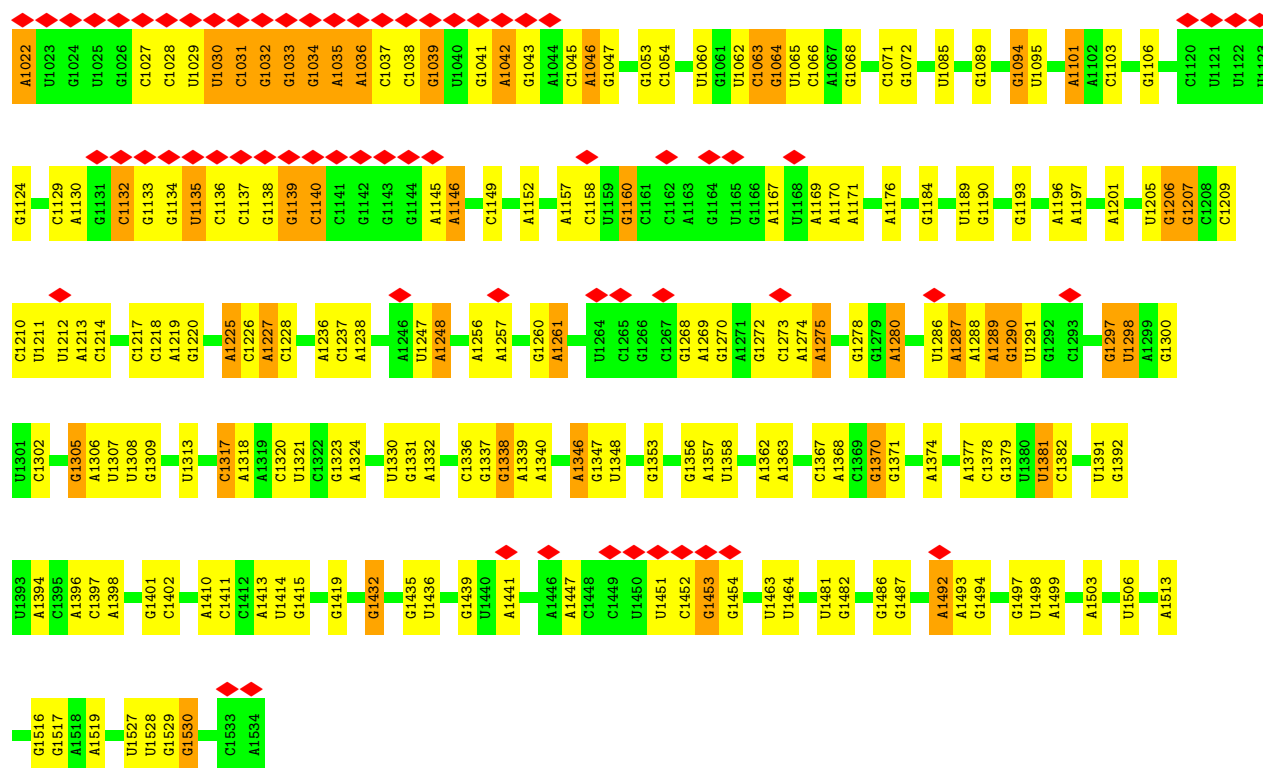


- Molecule 29: P-tRNA fMet

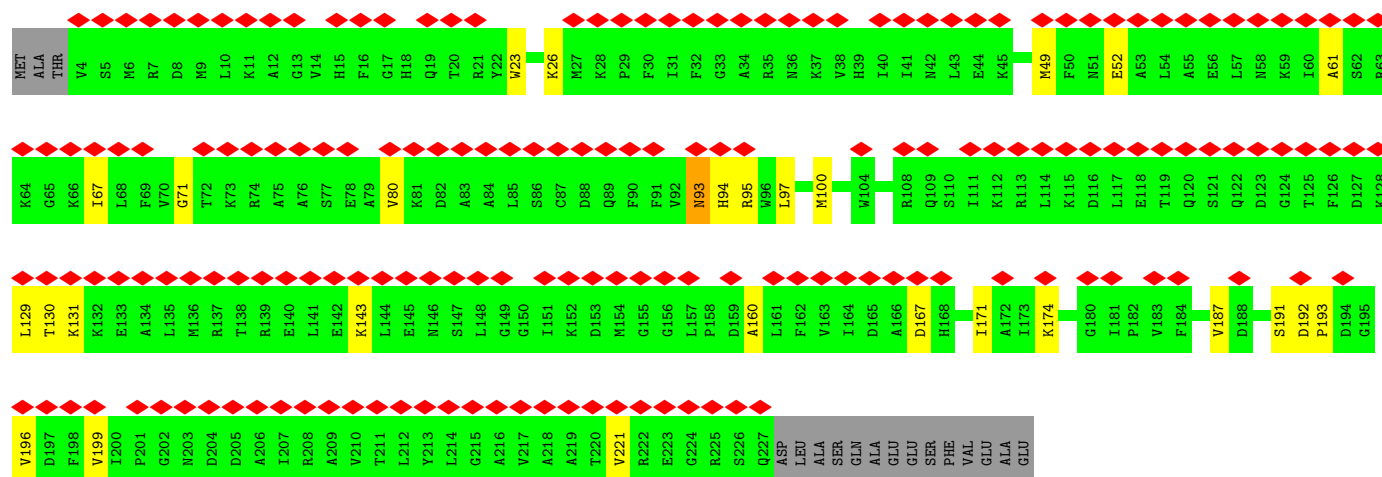
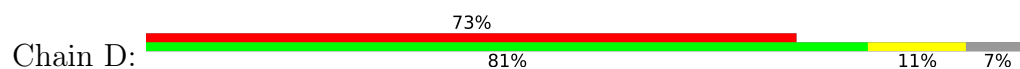


• Molecule 30: 16S ribosomal RNA

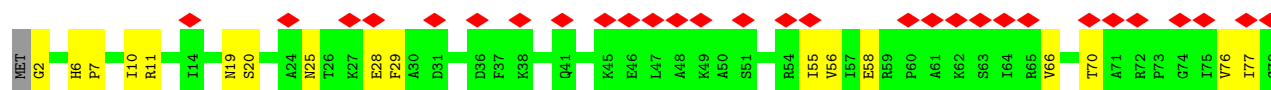


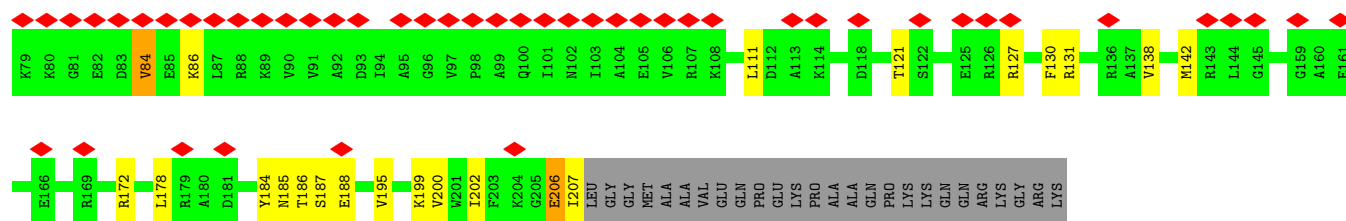


• Molecule 31: 30S ribosomal protein S2

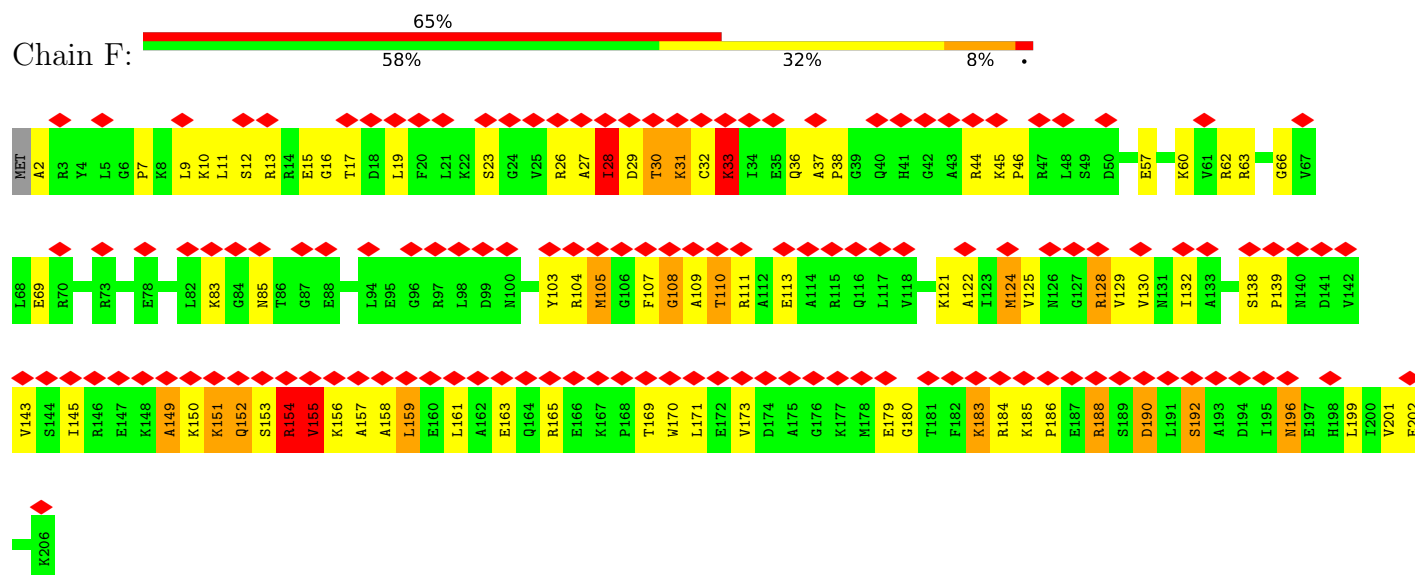


• Molecule 32: 30S ribosomal protein S3

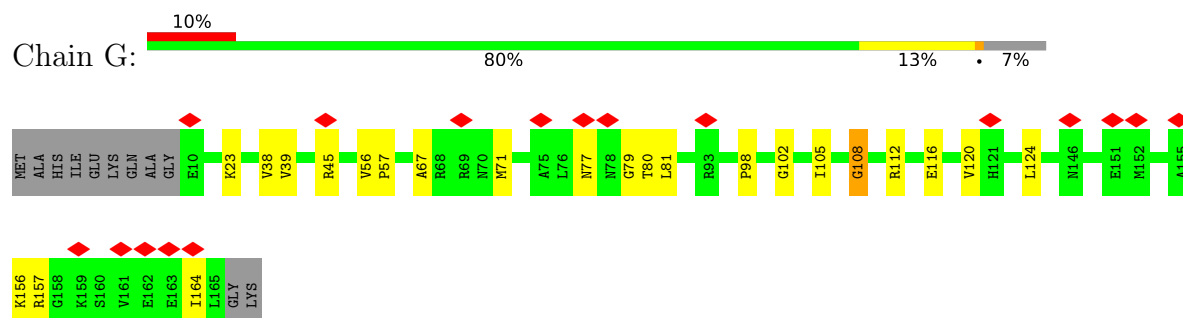




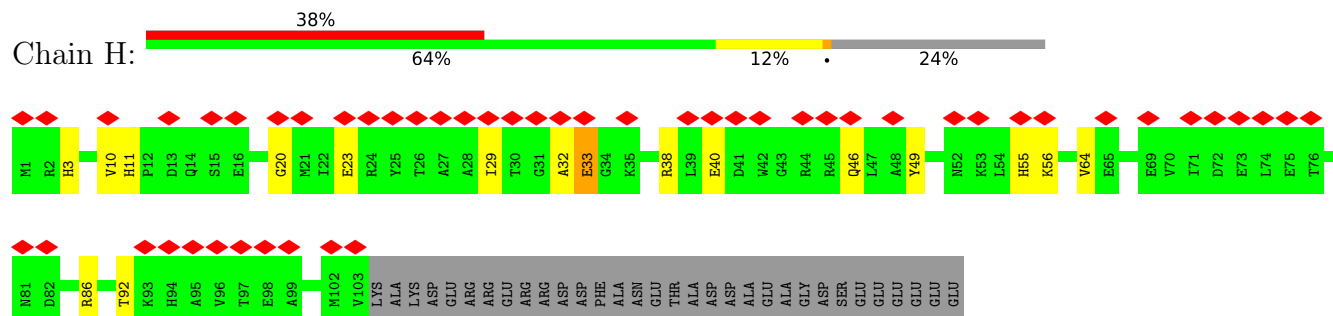
- Molecule 33: 30S ribosomal protein S4



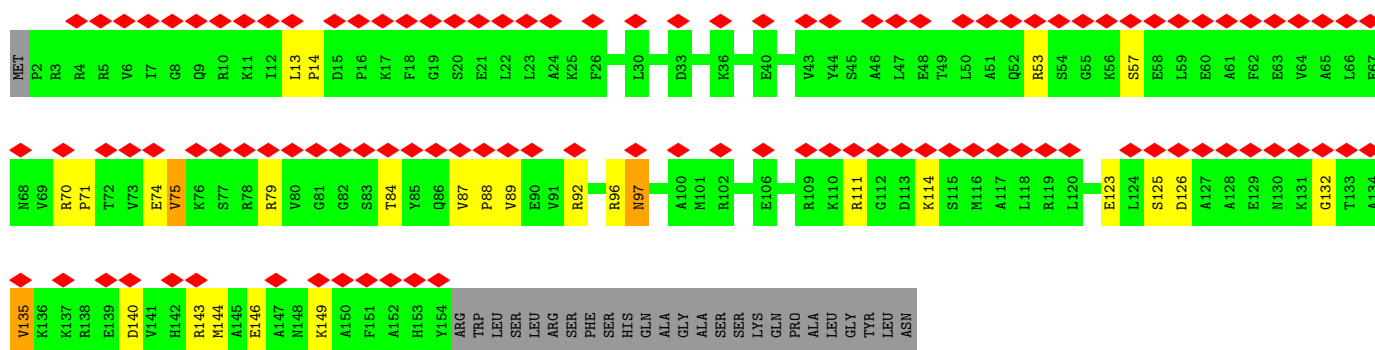
- Molecule 34: 30S ribosomal protein S5



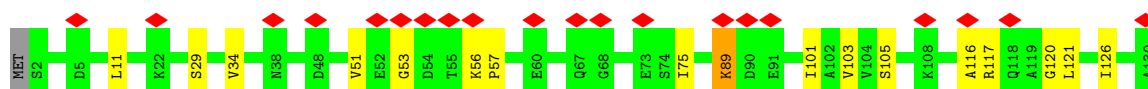
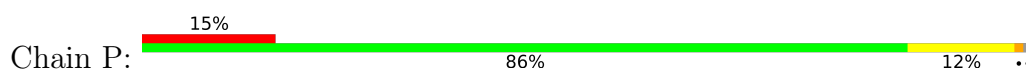
- Molecule 35: 30S ribosomal protein S6



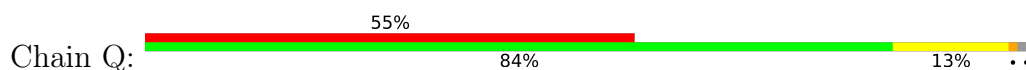
- Molecule 36: 30S ribosomal protein S7



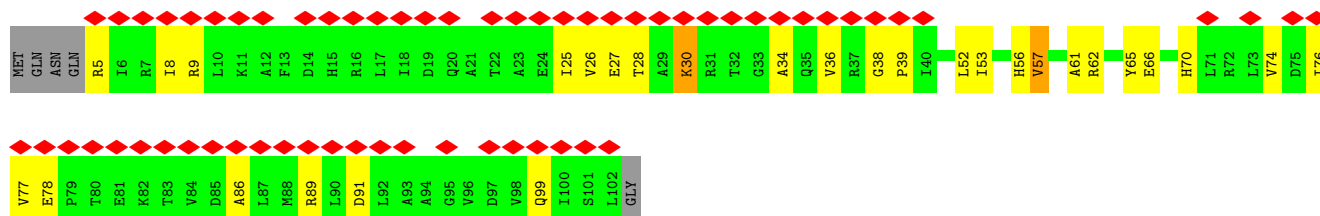
• Molecule 37: 30S ribosomal protein S8



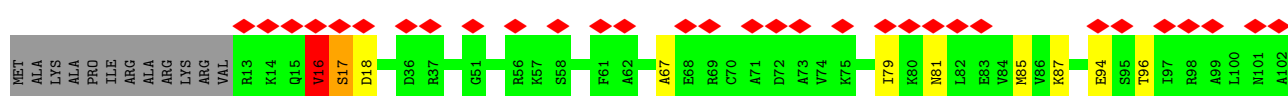
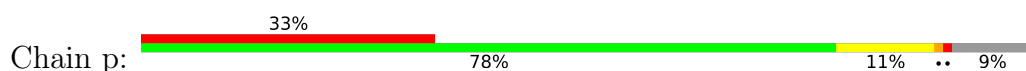
• Molecule 38: 30S ribosomal protein S9

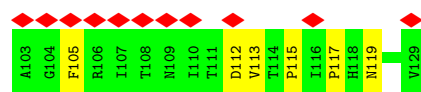


• Molecule 39: 30S ribosomal protein S10

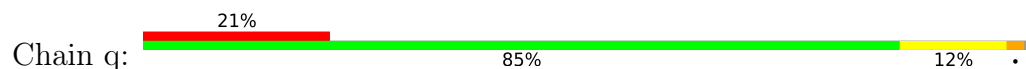


• Molecule 40: 30S ribosomal protein S11

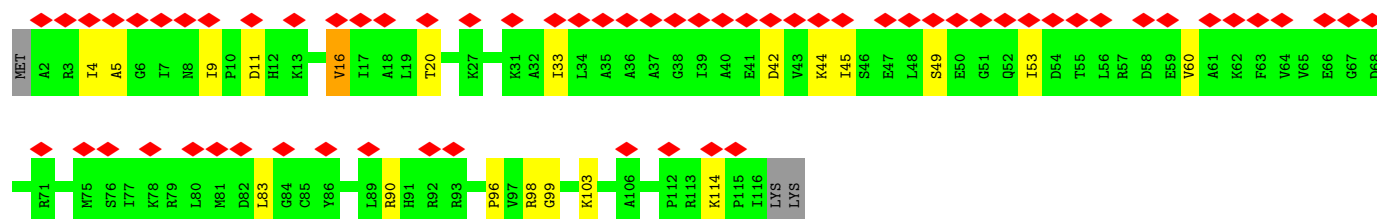
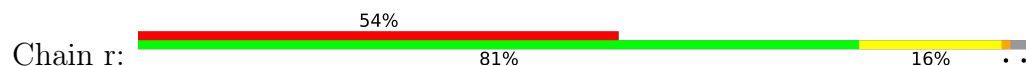




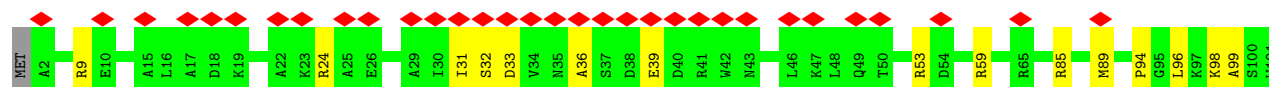
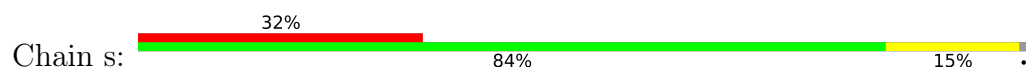
- Molecule 41: 30S ribosomal protein S12



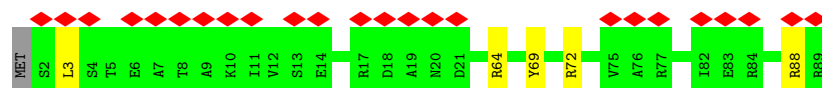
- Molecule 42: 30S ribosomal protein S13



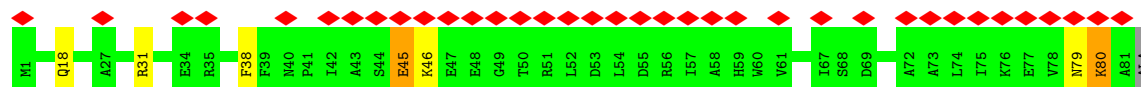
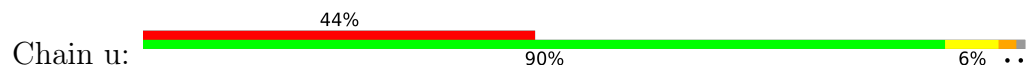
- Molecule 43: 30S ribosomal protein S14



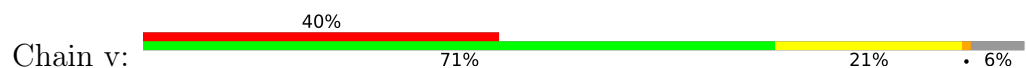
- Molecule 44: 30S ribosomal protein S15

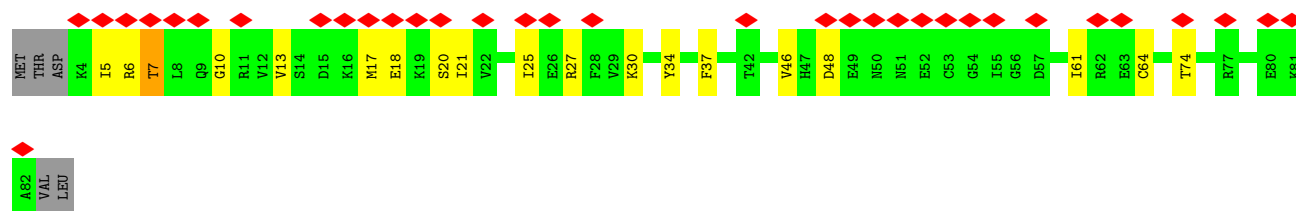


- Molecule 45: 30S ribosomal protein S16

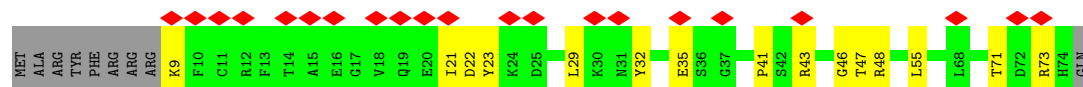


- Molecule 46: 30S ribosomal protein S17

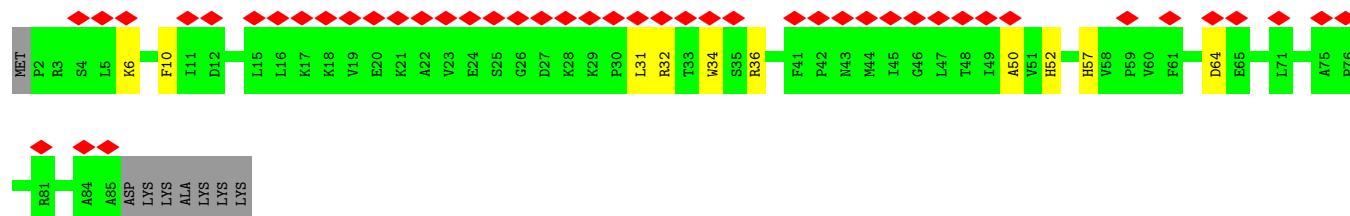
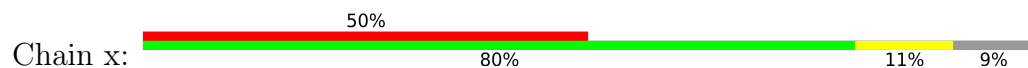




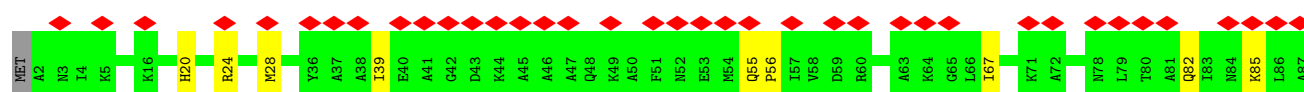
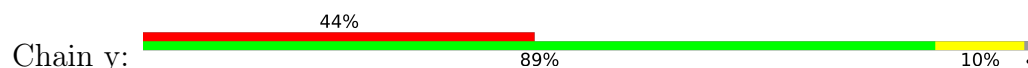
- Molecule 47: 30S ribosomal protein S18



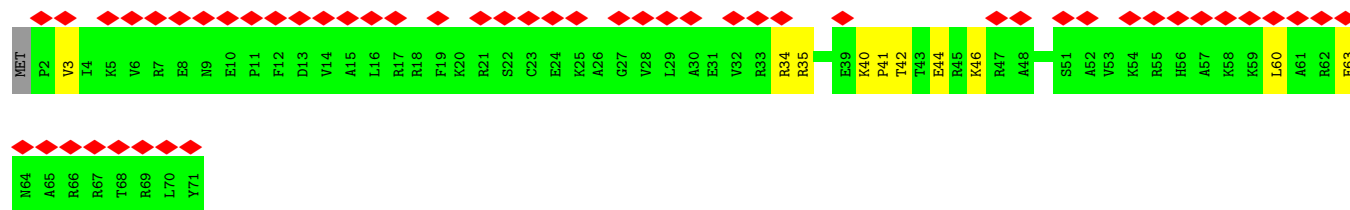
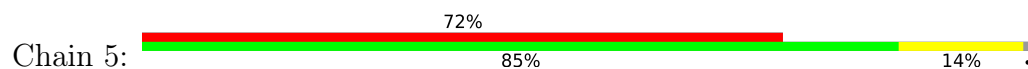
- Molecule 48: 30S ribosomal protein S19



- Molecule 49: 30S ribosomal protein S20



- Molecule 50: 30S ribosomal protein S21



- Molecule 51: messenger RNA



● Molecule 52: Myxovalargin B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	376564	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 ($e^-/\text{\AA}^2$)	2.5	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.186	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	379.08, 379.08, 379.08	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AG2, PSU, 2MA, OMC, ALQ, 5MC, SPD, IB9, DHV, RXL, RX9, ZN, OMG, OMU, 5MU, 1MG, DVA, DAR, MAA, FME, 2MG, DAL

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	I	0.24	0/69266	0.36	0/108061
2	J	0.22	0/2828	0.39	0/4410
3	K	0.20	0/2121	0.38	0/2852
4	L	0.19	0/1586	0.39	0/2134
5	M	0.18	0/1571	0.36	0/2113
6	O	0.14	0/1343	0.35	0/1816
7	R	0.18	0/1152	0.36	0/1551
8	S	0.19	0/947	0.38	0/1268
9	T	0.21	0/1062	0.39	0/1413
10	U	0.19	0/1093	0.37	0/1460
11	V	0.20	0/973	0.34	0/1301
12	W	0.16	0/902	0.39	0/1209
13	X	0.17	0/929	0.37	0/1242
14	Y	0.21	0/960	0.39	0/1278
15	Z	0.18	0/829	0.42	0/1107
16	a	0.20	0/864	0.41	0/1156
17	b	0.18	0/744	0.38	0/994
18	c	0.15	0/787	0.39	0/1051
19	d	0.17	0/766	0.41	0/1025
20	e	0.18	0/576	0.36	0/762
21	f	0.17	0/635	0.34	0/848
22	g	0.16	0/502	0.43	0/667
23	h	0.16	0/453	0.34	0/605
24	i	0.19	0/450	0.39	0/599
25	j	0.18	0/416	0.41	0/554
26	k	0.20	0/380	0.35	0/498
27	l	0.21	0/513	0.39	0/676
28	m	0.21	0/303	0.38	0/397
29	n	0.72	0/1813	1.45	73/2825 (2.6%)
30	C	0.25	0/36502	0.49	0/56940
31	D	0.15	0/1784	0.37	0/2403

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	E	0.15	0/1651	0.35	0/2225
33	F	0.19	0/1665	0.49	0/2227
34	G	0.16	0/1165	0.36	0/1568
35	H	0.16	0/858	0.38	0/1160
36	N	0.15	0/1219	0.37	0/1635
37	P	0.15	0/989	0.34	0/1326
38	Q	0.17	0/1034	0.36	0/1375
39	o	0.17	0/796	0.40	0/1077
40	p	0.20	0/893	0.44	0/1205
41	q	0.16	0/969	0.38	0/1300
42	r	0.15	0/900	0.37	0/1204
43	s	0.16	0/817	0.33	0/1088
44	t	0.16	0/722	0.30	0/964
45	u	0.17	0/653	0.39	0/877
46	v	0.16	0/650	0.38	0/871
47	w	0.18	0/553	0.37	0/742
48	x	0.14	0/685	0.36	0/922
49	y	0.14	0/676	0.33	0/895
50	5	0.17	0/597	0.34	0/792
51	6	0.34	0/72	0.45	0/110
52	z	0.18	0/10	0.73	0/11
All	All	0.24	0/152624	0.43	73/228789 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
39	o	0	1
52	z	0	1
All	All	0	2

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	70	C	P-O3'-C3'	-9.93	105.31	120.20
29	n	64	G	P-O3'-C3'	-9.70	105.65	120.20
29	n	51	U	P-O3'-C3'	-9.46	106.02	120.20
29	n	12	G	P-O3'-C3'	-9.15	106.48	120.20
29	n	71	G	P-O3'-C3'	-8.89	106.86	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	55	U	P-O3'-C3'	-8.75	107.08	120.20
29	n	17	C	P-O3'-C3'	-8.68	107.17	120.20
29	n	54	G	P-O3'-C3'	-8.64	107.24	120.20
29	n	8	U	P-O3'-C3'	-8.62	107.27	120.20
29	n	36	A	P-O3'-C3'	-8.38	107.62	120.20
29	n	69	C	P-O3'-C3'	-8.25	107.83	120.20
29	n	72	C	P-O3'-C3'	-8.23	107.85	120.20
29	n	62	C	P-O3'-C3'	-8.20	107.90	120.20
29	n	28	U	P-O3'-C3'	-8.19	107.92	120.20
29	n	22	A	P-O3'-C3'	-8.18	107.93	120.20
29	n	57	C	P-O3'-C3'	-8.07	108.09	120.20
29	n	66	C	P-O3'-C3'	-8.06	108.11	120.20
29	n	74	A	P-O3'-C3'	-8.05	108.13	120.20
29	n	37	U	P-O3'-C3'	-8.03	108.15	120.20
29	n	52	C	P-O3'-C3'	-7.96	108.26	120.20
29	n	19	G	P-O3'-C3'	-7.91	108.33	120.20
29	n	26	C	P-O3'-C3'	-7.89	108.36	120.20
29	n	3	C	P-O3'-C3'	-7.88	108.38	120.20
29	n	13	C	P-O3'-C3'	-7.80	108.50	120.20
29	n	4	G	P-O3'-C3'	-7.80	108.50	120.20
29	n	56	U	P-O3'-C3'	-7.80	108.50	120.20
29	n	43	G	P-O3'-C3'	-7.74	108.58	120.20
29	n	46	G	P-O3'-C3'	-7.68	108.68	120.20
29	n	32	G	P-O3'-C3'	-7.67	108.69	120.20
29	n	9	G	P-O3'-C3'	-7.63	108.75	120.20
29	n	49	C	P-O3'-C3'	-7.60	108.80	120.20
29	n	24	C	P-O3'-C3'	-7.55	108.87	120.20
29	n	75	C	P-O3'-C3'	-7.46	109.00	120.20
29	n	27	G	P-O3'-C3'	-7.41	109.09	120.20
29	n	50	G	P-O3'-C3'	-7.39	109.11	120.20
29	n	53	G	P-O3'-C3'	-7.36	109.16	120.20
29	n	31	G	P-O3'-C3'	-7.34	109.20	120.20
29	n	29	C	P-O3'-C3'	-7.26	109.31	120.20
29	n	61	U	P-O3'-C3'	-7.20	109.40	120.20
29	n	23	G	P-O3'-C3'	-7.15	109.47	120.20
29	n	68	C	P-O3'-C3'	-7.13	109.50	120.20
29	n	67	C	P-O3'-C3'	-7.13	109.51	120.20
29	n	7	G	P-O3'-C3'	-7.12	109.52	120.20
29	n	38	A	P-O3'-C3'	-7.09	109.57	120.20
29	n	30	G	P-O3'-C3'	-7.07	109.60	120.20
29	n	35	C	P-O3'-C3'	-6.97	109.75	120.20
29	n	11	A	P-O3'-C3'	-6.97	109.75	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	45	A	P-O3'-C3'	-6.95	109.77	120.20
29	n	48	U	P-O3'-C3'	-6.93	109.80	120.20
29	n	65	G	P-O3'-C3'	-6.90	109.86	120.20
29	n	2	G	P-O3'-C3'	-6.86	109.91	120.20
29	n	44	A	P-O3'-C3'	-6.83	109.96	120.20
29	n	25	U	P-O3'-C3'	-6.75	110.08	120.20
29	n	5	G	P-O3'-C3'	-6.68	110.18	120.20
29	n	41	C	P-O3'-C3'	-6.62	110.27	120.20
29	n	15	G	P-O3'-C3'	-6.60	110.30	120.20
29	n	73	A	P-O3'-C3'	-6.57	110.34	120.20
29	n	34	U	P-O3'-C3'	-6.53	110.40	120.20
29	n	60	A	P-O3'-C3'	-6.53	110.40	120.20
29	n	18	U	P-O3'-C3'	-6.46	110.50	120.20
29	n	39	A	P-O3'-C3'	-6.45	110.52	120.20
29	n	10	G	P-O3'-C3'	-6.37	110.65	120.20
29	n	14	A	P-O3'-C3'	-6.27	110.80	120.20
29	n	47	G	P-O3'-C3'	-6.16	110.96	120.20
29	n	59	A	P-O3'-C3'	-6.04	111.15	120.20
29	n	6	G	P-O3'-C3'	-5.79	111.52	120.20
29	n	58	A	P-O3'-C3'	-5.59	111.82	120.20
29	n	40	C	P-O3'-C3'	-5.57	111.84	120.20
29	n	21	U	P-O3'-C3'	-5.52	111.92	120.20
29	n	16	C	P-O3'-C3'	-5.30	112.25	120.20
29	n	33	C	P-O3'-C3'	-5.28	112.28	120.20
29	n	20	G	P-O3'-C3'	-5.24	112.34	120.20
29	n	77	A	C3'-C2'-C1'	5.05	106.55	101.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	o	38	GLY	Peptide
52	z	15	DHV	Peptide

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	I	62225	0	31309	373	0
2	J	2529	0	1280	11	0
3	K	2082	0	2154	23	0
4	L	1565	0	1616	9	0
5	M	1552	0	1619	12	0
6	O	1323	0	1371	13	0
7	R	1129	0	1162	12	0
8	S	938	0	1012	12	0
9	T	1053	0	1129	15	0
10	U	1074	0	1157	9	0
11	V	960	0	1000	6	0
12	W	892	0	923	5	0
13	X	917	0	962	10	0
14	Y	947	0	1019	12	0
15	Z	816	0	839	10	0
16	a	857	0	922	16	0
17	b	738	0	807	4	0
18	c	779	0	831	10	0
19	d	753	0	780	8	0
20	e	569	0	581	2	0
21	f	625	0	652	5	0
22	g	501	0	531	9	0
23	h	449	0	488	3	0
24	i	444	0	458	10	0
25	j	409	0	440	5	0
26	k	377	0	418	3	0
27	l	504	0	572	11	0
28	m	302	0	341	4	0
29	n	1623	0	824	98	0
30	C	32599	0	16405	328	0
31	D	1753	0	1780	13	0
32	E	1624	0	1696	18	0
33	F	1643	0	1707	79	0
34	G	1152	0	1196	13	0
35	H	839	0	833	9	0
36	N	1203	0	1254	17	0
37	P	979	0	1031	10	0
38	Q	1022	0	1070	15	0
39	o	786	0	828	17	0
40	p	877	0	887	11	0
41	q	955	0	1016	11	0
42	r	891	0	952	11	0
43	s	805	0	844	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	t	714	0	734	2	0
45	u	643	0	661	4	0
46	v	641	0	682	10	0
47	w	544	0	565	9	0
48	x	668	0	693	5	0
49	y	670	0	719	4	0
50	5	589	0	629	6	0
51	6	65	0	33	2	0
52	z	118	0	99	8	0
53	5	1	0	0	0	0
53	6	1	0	0	0	0
53	C	87	0	0	0	0
53	G	1	0	0	0	0
53	I	136	0	0	0	0
53	J	2	0	0	0	0
53	K	1	0	0	0	0
53	T	1	0	0	0	0
53	V	1	0	0	0	0
53	a	2	0	0	0	0
53	d	1	0	0	0	0
53	h	1	0	0	0	0
53	q	1	0	0	0	0
53	s	1	0	0	0	0
54	m	1	0	0	0	0
55	n	10	0	10	6	0
56	C	20	0	38	5	0
57	I	18	0	0	1	0
57	z	10	0	0	0	0
All	All	141008	0	93559	1203	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 5.

All (1203) 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)
55:n:101:FME:HG2	52:z:5:DVA:HG22	1.51	0.93
30:C:1206:G:H3'	30:C:1207:G:H8	1.38	0.89
29:n:16:C:H4'	29:n:60:A:H2	1.37	0.87
29:n:63:C:H2'	29:n:64:G:C8	2.12	0.84
29:n:22:A:H61	29:n:47:G:H2'	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:n:67:C:H2'	29:n:68:C:H1'	1.62	0.81
29:n:16:C:H4'	29:n:60:A:C2	2.17	0.80
29:n:24:C:H2'	29:n:25:U:C6	2.16	0.80
30:C:718:A:O2'	50:5:35:ARG:NH2	2.16	0.79
30:C:1206:G:H3'	30:C:1207:G:C8	2.20	0.75
29:n:44:A:H2'	29:n:45:A:C8	2.21	0.75
30:C:618:C:H5'	30:C:619:U:H5''	1.71	0.72
29:n:19:G:H4'	29:n:61:U:O2	1.89	0.71
30:C:429:U:O2'	33:F:26:ARG:NH2	2.23	0.71
1:I:1173:U:H2'	1:I:1174:U:H4'	1.73	0.71
29:n:45:A:H2'	29:n:46:G:C8	2.26	0.71
29:n:9:G:H5'	29:n:47:G:H1'	1.74	0.69
36:N:79:ARG:HA	36:N:84:THR:HA	1.75	0.69
52:z:5:DVA:HG13	52:z:6:DVA:HG13	1.73	0.68
29:n:63:C:H2'	29:n:64:G:H8	1.56	0.68
30:C:453:G:N7	56:C:1688:SPD:N6	2.41	0.68
30:C:1060:U:OP1	43:s:85:ARG:NH2	2.27	0.68
30:C:717:U:H4'	40:p:119:ASN:HD22	1.59	0.68
30:C:1530:G:O6	50:5:46:LYS:NZ	2.27	0.68
29:n:22:A:N6	29:n:47:G:H2'	2.09	0.67
29:n:27:G:H22	29:n:45:A:H2	1.42	0.66
55:n:101:FME:HG2	52:z:5:DVA:CG2	2.24	0.66
30:C:717:U:H4'	40:p:119:ASN:ND2	2.10	0.66
29:n:9:G:H21	29:n:46:G:H3'	1.60	0.66
29:n:67:C:H2'	29:n:68:C:C1'	2.25	0.65
29:n:25:U:H2'	29:n:26:C:C6	2.32	0.65
36:N:53:ARG:NH2	36:N:125:SER:OG	2.29	0.65
29:n:19:G:H1	29:n:56:U:H6	1.43	0.65
30:C:127:G:O2'	46:v:6:ARG:NH1	2.30	0.65
34:G:105:ILE:O	34:G:112:ARG:NH2	2.28	0.65
1:I:2419:U:H4'	25:j:22:THR:HG21	1.79	0.65
29:n:17:C:H2'	29:n:18:U:C6	2.33	0.64
30:C:966:G:H2'	30:C:967:C:C6	2.31	0.64
1:I:2602:A:H3'	1:I:2603:G:H5''	1.80	0.64
33:F:62:ARG:O	33:F:66:GLY:N	2.31	0.64
30:C:1377:A:OP1	36:N:92:ARG:NH2	2.31	0.64
30:C:505:G:H5'	30:C:534:U:H2'	1.80	0.63
30:C:618:C:N4	30:C:621:A:OP2	2.32	0.63
30:C:429:U:H5'	33:F:31:LYS:HD3	1.79	0.63
33:F:12:SER:O	33:F:16:GLY:N	2.32	0.63
1:I:613:A:H3'	1:I:614:A:C5'	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:n:34:U:C5	38:Q:130:ARG:CZ	2.83	0.62
30:C:1287:A:N1	30:C:1370:G:N2	2.47	0.62
33:F:32:CYS:O	33:F:33:LYS:C	2.42	0.62
1:I:1116:G:H2'	1:I:1117:C:C6	2.35	0.62
29:n:51:U:H3	29:n:65:G:H1	1.47	0.62
30:C:515:G:H3'	30:C:516:U:H6	1.65	0.62
29:n:31:G:O2'	29:n:32:G:H5'	2.00	0.62
29:n:53:G:H2'	29:n:54:G:O4'	1.98	0.62
39:o:66:GLU:HB2	43:s:99:ALA:HB2	1.82	0.61
29:n:50:G:H2'	29:n:51:U:C6	2.35	0.61
30:C:1152:A:OP1	39:o:70:HIS:ND1	2.33	0.61
1:I:2405:G:O2'	1:I:2411:A:N6	2.33	0.60
1:I:1179:G:H3'	1:I:1180:U:H5''	1.83	0.60
56:C:1689:SPD:HN11	56:C:1689:SPD:H51	1.66	0.60
1:I:1645:G:H5''	1:I:1646:C:H5'	1.84	0.60
30:C:769:G:H4'	30:C:1513:A:H4'	1.82	0.59
29:n:49:C:H2'	29:n:60:A:H1'	1.84	0.59
30:C:202:G:H2'	30:C:203:G:C8	2.37	0.59
22:g:45:GLN:O	22:g:46:VAL:HB	2.01	0.59
1:I:807:U:OP2	9:T:41:ARG:NH2	2.36	0.59
35:H:32:ALA:O	35:H:33:GLU:HB2	2.02	0.59
29:n:36:A:OP2	38:Q:130:ARG:NH2	2.36	0.59
1:I:2796:U:H2'	1:I:2797:U:H2'	1.85	0.59
1:I:2210:U:H4'	1:I:2211:A:H5'	1.84	0.59
29:n:8:U:H5'	29:n:50:G:H5'	1.84	0.59
30:C:294:U:OP1	30:C:610:U:O2'	2.20	0.59
1:I:2318:G:O2'	1:I:2319:G:OP1	2.21	0.58
29:n:19:G:H21	29:n:59:A:H5'	1.66	0.58
33:F:150:LYS:O	33:F:152:GLN:N	2.36	0.58
14:Y:87:SER:HB3	15:Z:52:PRO:HD3	1.84	0.58
1:I:747:5MU:O2'	16:a:92:ARG:NH2	2.37	0.58
33:F:196:ASN:OD1	33:F:196:ASN:N	2.36	0.58
49:y:55:GLN:HB3	49:y:56:PRO:HD3	1.86	0.58
29:n:5:G:H2'	29:n:6:G:C8	2.39	0.57
30:C:1391:U:H2'	30:C:1392:G:C8	2.38	0.57
1:I:45:G:H5''	1:I:46:G:H5'	1.85	0.57
33:F:188:ARG:NH2	33:F:192:SER:O	2.38	0.57
1:I:1450:G:N2	1:I:1452:G:O6	2.37	0.57
29:n:53:G:H1	29:n:63:C:H42	1.51	0.57
6:O:149:ARG:HA	6:O:162:VAL:HB	1.87	0.57
29:n:10:G:H3'	29:n:11:A:H8	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:p:17:SER:HA	40:p:79:ILE:HA	1.87	0.57
30:C:405:U:O4	33:F:2:ALA:N	2.38	0.57
1:I:545:U:H2'	1:I:546:U:H4'	1.86	0.57
29:n:13:C:H2'	29:n:14:A:H5''	1.87	0.57
1:I:1178:C:N4	1:I:1179:G:O6	2.38	0.57
30:C:1346:A:OP1	38:Q:122:ARG:NH1	2.38	0.57
1:I:2161:C:H2'	1:I:2162:G:H5'	1.87	0.56
29:n:8:U:H1'	29:n:49:C:H1'	1.87	0.56
1:I:141:G:N3	1:I:141:G:H2'	2.20	0.56
1:I:495:G:N3	16:a:61:ASN:ND2	2.51	0.56
33:F:184:ARG:NH2	33:F:185:LYS:O	2.38	0.56
4:L:104:VAL:O	4:L:105:LYS:HB2	2.05	0.56
25:j:40:ASP:HB3	25:j:43:VAL:HG12	1.87	0.56
33:F:151:LYS:O	33:F:152:GLN:C	2.49	0.56
1:I:1309:G:H4'	26:k:7:PRO:HB2	1.88	0.56
1:I:2182:U:H2'	1:I:2183:A:C8	2.40	0.56
30:C:481:G:O2'	30:C:483:C:N4	2.39	0.56
30:C:1347:G:C8	38:Q:109:ARG:HB3	2.41	0.56
29:n:65:G:H2'	29:n:66:C:C6	2.40	0.55
33:F:45:LYS:H	33:F:45:LYS:HD3	1.70	0.55
12:W:33:ARG:O	12:W:34:HIS:HB2	2.07	0.55
29:n:28:U:H2'	29:n:29:C:C6	2.42	0.55
47:w:9:LYS:HA	47:w:46:GLY:HA3	1.88	0.55
48:x:50:ALA:HB1	48:x:57:HIS:HB3	1.88	0.55
30:C:94:G:C8	30:C:94:G:H5'	2.42	0.55
41:q:44:LYS:HB3	41:q:45:PRO:HD3	1.88	0.55
5:M:128:ALA:HB1	5:M:129:PRO:HD2	1.88	0.55
29:n:56:U:H5	29:n:59:A:OP2	1.90	0.55
30:C:418:C:H5''	30:C:419:C:H5'	1.88	0.55
30:C:464:U:H2'	30:C:465:A:H5''	1.88	0.55
9:T:77:ILE:HD13	9:T:108:ALA:HB1	1.89	0.55
15:Z:54:VAL:HG13	15:Z:57:GLY:H	1.71	0.55
30:C:1106:G:H5''	32:E:172:ARG:HG2	1.88	0.55
1:I:1026:G:H2'	1:I:1027:A:C8	2.42	0.55
3:K:29:PRO:HG2	3:K:34:LEU:HD11	1.89	0.55
1:I:2425:A:H4'	1:I:2426:A:O5'	2.07	0.54
1:I:2451:A:H1'	29:n:77:A:H2'	1.89	0.54
29:n:29:C:H2'	29:n:29:C:O2	2.07	0.54
33:F:31:LYS:HD2	33:F:31:LYS:N	2.23	0.54
1:I:864:G:O2'	1:I:914:G:O6	2.24	0.54
29:n:29:C:H42	29:n:43:G:H1	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:163:C:H2'	30:C:164:G:O4'	2.07	0.54
30:C:309:A:O2'	30:C:607:A:N1	2.36	0.54
30:C:575:G:O2'	30:C:821:G:OP2	2.22	0.54
30:C:1247:U:H2'	30:C:1248:A:H5''	1.90	0.54
1:I:898:C:H2'	1:I:899:A:O4'	2.08	0.54
1:I:157:C:H2'	1:I:158:U:O4'	2.08	0.54
39:o:26:VAL:HA	39:o:36:VAL:HG11	1.90	0.54
1:I:803:U:H2'	1:I:804:A:H5''	1.89	0.54
30:C:408:A:O2'	30:C:409:U:O2	2.13	0.54
1:I:1060:U:H1'	1:I:1062:G:H5'	1.89	0.54
1:I:528:A:H2'	1:I:529:A:H5''	1.90	0.53
9:T:63:LYS:HG2	27:l:13:ARG:HD2	1.90	0.53
29:n:68:C:H2'	29:n:68:C:O2	2.07	0.53
33:F:108:GLY:C	33:F:110:THR:H	2.15	0.53
33:F:153:SER:O	33:F:154:ARG:HB3	2.08	0.53
29:n:20:G:H3'	29:n:21:U:C5	2.44	0.53
30:C:660:C:H2'	30:C:661:G:O4'	2.07	0.53
34:G:45:ARG:HG2	34:G:71:MET:HE2	1.90	0.53
30:C:1062:U:H2'	30:C:1063:C:C6	2.43	0.53
45:u:45:GLU:O	45:u:46:LYS:HB2	2.08	0.53
1:I:870:U:H2'	1:I:871:U:H5'	1.90	0.53
1:I:2757:A:H2'	1:I:2758:A:H5''	1.91	0.53
7:R:4:PHE:O	14:Y:64:ARG:NH2	2.42	0.53
1:I:948:C:H1'	1:I:984:A:C8	2.44	0.53
30:C:425:G:N3	30:C:425:G:H2'	2.24	0.53
29:n:54:G:H2'	29:n:54:G:N3	2.22	0.53
30:C:515:G:H3'	30:C:516:U:C6	2.43	0.53
30:C:1005:A:C4	30:C:1006:G:H1'	2.43	0.52
29:n:20:G:H5'	29:n:61:U:H3	1.74	0.52
29:n:46:G:O5'	29:n:46:G:H8	1.92	0.52
1:I:2113:U:H3'	1:I:2114:A:H5''	1.91	0.52
29:n:54:G:H3'	29:n:55:U:H6	1.74	0.52
30:C:1149:C:O2'	30:C:1280:A:N1	2.40	0.52
1:I:2273:A:H2'	1:I:2274:A:C8	2.44	0.52
1:I:2638:G:O2'	1:I:2775:G:N2	2.42	0.52
30:C:25:C:H5'	30:C:524:G:H1'	1.92	0.52
1:I:2063:C:H4'	55:n:101:FME:SD	2.49	0.52
30:C:52:C:H5''	30:C:52:C:H6	1.75	0.52
1:I:910:A:H2'	1:I:911:A:C8	2.45	0.52
1:I:1087:G:H2'	1:I:1089:A:H5'	1.91	0.52
3:K:89:ALA:HB2	3:K:157:SER:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:n:35:C:H42	51:6:27:G:H1	1.58	0.52
30:C:273:U:O4	30:C:274:A:N6	2.43	0.52
35:H:29:ILE:HG21	35:H:64:VAL:HG21	1.91	0.52
29:n:9:G:C5'	29:n:47:G:H1'	2.40	0.52
30:C:946:A:H2'	30:C:947:G:C8	2.45	0.52
10:U:75:GLU:HB2	10:U:90:GLU:HG3	1.92	0.52
16:a:7:HIS:HB2	16:a:50:VAL:HG22	1.91	0.52
1:I:2:G:H2'	1:I:3:U:C6	2.45	0.51
1:I:248:G:O5'	1:I:249:C:H5''	2.10	0.51
1:I:554:U:H2'	1:I:555:G:O4'	2.10	0.51
6:O:123:ALA:HB2	6:O:133:LEU:HD23	1.90	0.51
29:n:11:A:H2'	29:n:11:A:N3	2.26	0.51
29:n:19:G:N2	29:n:59:A:OP2	2.42	0.51
30:C:411:A:H8	30:C:412:A:H2'	1.76	0.51
30:C:433:G:H3'	30:C:434:U:C5'	2.41	0.51
29:n:15:G:H2'	29:n:16:C:H5'	1.91	0.51
34:G:39:VAL:HG22	34:G:67:ALA:HB1	1.93	0.51
1:I:813:U:H2'	1:I:814:C:C6	2.46	0.51
3:K:232:HIS:HA	3:K:242:LYS:HD2	1.93	0.51
30:C:792:A:H4'	30:C:793:U:O5'	2.11	0.51
30:C:1034:G:H2'	30:C:1035:A:C8	2.45	0.51
33:F:33:LYS:O	33:F:36:GLN:N	2.40	0.51
2:J:9:G:O2'	12:W:45:SER:HA	2.10	0.51
9:T:78:ARG:HG2	9:T:113:ALA:HB3	1.93	0.51
56:C:1689:SPD:H51	56:C:1689:SPD:N1	2.25	0.51
39:o:36:VAL:HB	39:o:76:ILE:HD13	1.93	0.51
1:I:2115:G:H2'	1:I:2117:A:OP2	2.10	0.51
16:a:59:GLU:HA	16:a:64:ALA:HA	1.92	0.51
30:C:419:C:H2'	30:C:419:C:O2	2.10	0.51
1:I:639:U:H2'	1:I:640:C:C6	2.46	0.51
30:C:1132:C:N4	30:C:1133:G:O6	2.43	0.51
33:F:15:GLU:OE1	33:F:63:ARG:NH1	2.44	0.51
1:I:892:A:H2'	1:I:893:C:C6	2.46	0.50
1:I:1722:A:H2'	1:I:1723:G:O4'	2.11	0.50
7:R:140:LEU:HG	7:R:142:ILE:HG22	1.93	0.50
8:S:71:ARG:HB3	8:S:72:PRO:HD2	1.94	0.50
30:C:718:A:OP2	30:C:720:C:N4	2.44	0.50
30:C:751:U:H2'	30:C:752:G:O4'	2.11	0.50
1:I:1105:U:H2'	1:I:1106:G:H8	1.76	0.50
30:C:482:A:H2'	30:C:483:C:O4'	2.11	0.50
35:H:20:GLY:O	35:H:23:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1430:G:H2'	1:I:1431:A:O4'	2.11	0.50
15:Z:49:ILE:HG13	15:Z:49:ILE:O	2.11	0.50
29:n:44:A:H2'	29:n:45:A:H8	1.73	0.50
30:C:74:A:H2'	30:C:75:G:O4'	2.12	0.50
1:I:265:A:H4'	1:I:266:G:H5'	1.94	0.50
1:I:1779:U:H5	1:I:1784:A:N7	2.08	0.50
1:I:1817:G:H2'	1:I:1818:U:H5'	1.94	0.50
29:n:45:A:H2'	29:n:46:G:H8	1.75	0.50
1:I:356:G:H2'	1:I:357:C:C6	2.46	0.50
1:I:1182:G:H2'	1:I:1183:U:O4'	2.12	0.50
29:n:21:U:H6	29:n:21:U:O5'	1.94	0.50
29:n:45:A:H8	29:n:45:A:O5'	1.95	0.50
30:C:362:G:N2	30:C:365:U:OP2	2.39	0.50
30:C:371:A:H2'	30:C:372:C:O4'	2.11	0.50
30:C:469:C:H2'	30:C:470:C:C6	2.47	0.50
30:C:1010:U:H2'	30:C:1011:C:C6	2.46	0.50
30:C:1032:G:C5	30:C:1033:G:H1'	2.47	0.50
1:I:784:G:H5'	1:I:785:G:OP1	2.12	0.50
1:I:2150:C:H2'	1:I:2151:U:C6	2.47	0.50
13:X:106:LYS:HD2	30:C:1432:G:O5'	2.11	0.50
31:D:61:ALA:HB2	31:D:221:VAL:HG13	1.94	0.50
1:I:1589:U:H2'	1:I:1590:A:C8	2.47	0.50
1:I:1271:G:O3'	1:I:1272:A:H4'	2.12	0.50
17:b:13:ALA:HB1	22:g:33:ALA:CB	2.42	0.50
19:d:30:ILE:HA	19:d:91:PHE:O	2.11	0.50
36:N:75:VAL:HA	36:N:87:VAL:O	2.12	0.50
1:I:360:U:H2'	1:I:361:G:C4	2.47	0.49
1:I:1177:G:H2'	1:I:1178:C:C6	2.47	0.49
1:I:1666:G:C2'	1:I:1667:G:H5'	2.41	0.49
1:I:2188:U:H3'	1:I:2189:U:H5''	1.94	0.49
1:I:2320:U:H4'	1:I:2321:U:H5''	1.93	0.49
30:C:1236:A:H2'	30:C:1237:C:C6	2.47	0.49
1:I:24:G:O2'	16:a:78:GLU:O	2.30	0.49
7:R:99:ARG:HE	7:R:99:ARG:HA	1.75	0.49
18:c:3:ALA:O	18:c:4:LYS:HB2	2.12	0.49
23:h:3:LYS:O	23:h:4:THR:HB	2.12	0.49
30:C:350:G:H2'	30:C:351:G:C8	2.47	0.49
30:C:407:U:O2'	30:C:408:A:H5'	2.12	0.49
30:C:1035:A:H4'	30:C:1036:A:OP1	2.12	0.49
36:N:111:ARG:NH2	36:N:126:ASP:OD2	2.43	0.49
40:p:87:LYS:HB2	40:p:113:VAL:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:645:C:H2'	1:I:647:G:C8	2.47	0.49
1:I:2777:G:H5'	1:I:2781:A:H1'	1.93	0.49
1:I:1059:G:C8	1:I:1060:U:H2'	2.47	0.49
39:o:77:VAL:HG12	39:o:78:GLU:HG2	1.94	0.49
40:p:16:VAL:HG22	40:p:18:ASP:H	1.77	0.49
47:w:71:THR:HG23	47:w:73:ARG:H	1.78	0.49
3:K:140:THR:HG23	3:K:161:TYR:HB2	1.93	0.49
30:C:171:A:H2'	30:C:172:A:C8	2.46	0.49
32:E:186:THR:HG22	32:E:199:LYS:HG2	1.95	0.49
1:I:1428:C:C5	1:I:1569:A:H5''	2.47	0.49
1:I:2123:G:H2'	1:I:2124:G:O4'	2.13	0.49
30:C:428:G:H4'	30:C:429:U:O5'	2.12	0.49
31:D:93:ASN:H	31:D:93:ASN:HD22	1.61	0.49
1:I:322:A:H5'	1:I:340:A:H1'	1.94	0.49
1:I:534:U:O2'	14:Y:49:ASP:OD2	2.30	0.49
1:I:61:C:O4'	22:g:40:SER:HB2	2.11	0.49
1:I:1038:G:H2'	1:I:1039:A:C8	2.48	0.49
1:I:2291:U:H2'	1:I:2292:U:C6	2.47	0.49
30:C:439:U:H4'	33:F:121:LYS:NZ	2.27	0.49
37:P:29:SER:HB3	37:P:57:PRO:HB2	1.94	0.49
1:I:44:A:H2'	1:I:45:G:O4'	2.13	0.49
1:I:740:C:H5'	1:I:1784:A:H3'	1.93	0.49
1:I:870:U:C2'	1:I:871:U:H5'	2.43	0.49
1:I:871:U:H2'	1:I:872:U:C6	2.48	0.49
30:C:432:A:H2'	30:C:433:G:O4'	2.13	0.49
30:C:820:U:H4'	30:C:821:G:OP2	2.12	0.49
30:C:901:A:O2'	30:C:1513:A:OP1	2.24	0.49
30:C:967:C:OP1	30:C:969:A:H5'	2.13	0.49
30:C:1323:G:H2'	30:C:1324:A:C8	2.47	0.49
30:C:1401:G:H2'	30:C:1402:C:O4'	2.13	0.49
1:I:2058:A:C2	52:z:12:DVA:HG23	2.47	0.48
1:I:2063:C:H1'	55:n:101:FME:N	2.28	0.48
1:I:2137:U:H2'	1:I:2138:G:C8	2.48	0.48
14:Y:94:ILE:HD12	15:Z:13:ARG:HB2	1.94	0.48
30:C:431:A:HO2'	30:C:432:A:H8	1.60	0.48
30:C:1189:U:OP1	43:s:98:LYS:NZ	2.46	0.48
30:C:1435:G:H2'	30:C:1436:U:C6	2.48	0.48
29:n:60:A:H2'	29:n:60:A:N3	2.27	0.48
30:C:451:A:H4'	30:C:452:A:O4'	2.13	0.48
30:C:600:A:H4'	37:P:120:GLY:O	2.12	0.48
33:F:13:ARG:HB2	33:F:38:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:p:16:VAL:HG13	40:p:17:SER:H	1.78	0.48
1:I:404:A:H4'	1:I:405:U:O5'	2.12	0.48
1:I:1581:G:C2	1:I:1582:C:H1'	2.49	0.48
11:V:100:CYS:HA	24:i:43:ILE:HG12	1.96	0.48
45:u:18:GLN:HA	45:u:38:PHE:HA	1.95	0.48
50:5:40:LYS:HD2	50:5:42:THR:HG22	1.95	0.48
1:I:2112:G:H5'	1:I:2112:G:H8	1.78	0.48
1:I:2177:C:H2'	1:I:2178:C:C6	2.49	0.48
5:M:76:PRO:HA	5:M:82:GLY:HA3	1.94	0.48
25:j:25:LYS:HD2	25:j:52:ALA:HB1	1.94	0.48
29:n:24:C:H2'	29:n:25:U:H6	1.73	0.48
29:n:26:C:H2'	29:n:27:G:O4'	2.13	0.48
33:F:149:ALA:O	33:F:151:LYS:HG2	2.12	0.48
29:n:52:C:H2'	29:n:53:G:C8	2.49	0.48
30:C:436:C:O3'	33:F:153:SER:HB2	2.14	0.48
30:C:1401:G:C2	30:C:1402:C:H1'	2.49	0.48
1:I:1542:U:H2'	1:I:1543:G:O4'	2.14	0.48
1:I:2309:A:H2'	1:I:2310:C:C6	2.48	0.48
18:c:16:GLY:O	18:c:17:LYS:HB3	2.13	0.48
30:C:590:U:H2'	30:C:591:U:C6	2.49	0.48
38:Q:118:LEU:HD22	38:Q:124:ARG:HG2	1.95	0.48
1:I:1013:C:H2'	1:I:1014:A:C8	2.48	0.48
6:O:94:TYR:HA	6:O:106:SER:O	2.14	0.48
30:C:426:U:OP1	33:F:33:LYS:HE3	2.14	0.48
36:N:74:GLU:HG3	36:N:89:VAL:HG23	1.96	0.48
40:p:87:LYS:HG3	40:p:115:PRO:HD3	1.95	0.48
1:I:1100:C:H2'	1:I:1101:U:C6	2.48	0.48
30:C:538:G:OP1	41:q:110:ARG:HD2	2.14	0.48
30:C:1068:G:N7	30:C:1094:G:H2'	2.28	0.48
32:E:200:VAL:HG12	32:E:202:ILE:HG13	1.94	0.48
33:F:26:ARG:HD3	33:F:26:ARG:H	1.78	0.48
33:F:44:ARG:O	33:F:46:PRO:HD3	2.13	0.48
36:N:13:LEU:HD12	36:N:14:PRO:HD2	1.96	0.48
37:P:34:VAL:HG22	37:P:51:VAL:HG21	1.95	0.48
1:I:1138:G:H2'	1:I:1139:G:O4'	2.14	0.48
30:C:190:A:C4	30:C:191:G:H1'	2.49	0.48
30:C:458:U:H2'	30:C:458:U:O2	2.14	0.48
1:I:215:G:H4'	1:I:216:A:H4'	1.96	0.48
1:I:1357:C:H2'	1:I:1358:G:O4'	2.14	0.48
13:X:31:TRP:CE3	13:X:38:LYS:HD2	2.49	0.48
19:d:6:ALA:HB3	19:d:63:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:k:46:LYS:HD2	26:k:46:LYS:N	2.29	0.48
30:C:418:C:OP2	30:C:418:C:H3'	2.13	0.48
33:F:150:LYS:N	33:F:150:LYS:HD2	2.29	0.48
1:I:2114:A:H2'	1:I:2166:U:O2'	2.14	0.47
25:j:6:ARG:HG2	25:j:24:THR:HB	1.95	0.47
30:C:1060:U:H4'	39:o:53:ILE:HG13	1.96	0.47
1:I:1923:U:H5''	29:n:25:U:O2'	2.14	0.47
1:I:2071:A:H2'	1:I:2072:C:C6	2.50	0.47
1:I:2552:OMU:HM23	1:I:2554:U:C6	2.48	0.47
30:C:1498:U:H4'	30:C:1519:A:H2	1.79	0.47
47:w:23:TYR:HA	47:w:29:LEU:HD11	1.96	0.47
16:a:66:ILE:HG12	16:a:66:ILE:O	2.13	0.47
20:e:41:ARG:HH11	20:e:41:ARG:HA	1.80	0.47
30:C:299:G:H2'	30:C:300:A:C8	2.49	0.47
30:C:1356:G:H2'	30:C:1357:A:C8	2.49	0.47
33:F:103:TYR:HA	33:F:108:GLY:HA3	1.96	0.47
1:I:1068:G:O3'	1:I:1070:A:N6	2.47	0.47
33:F:13:ARG:NE	33:F:32:CYS:O	2.47	0.47
1:I:588:U:H2'	1:I:589:U:C6	2.49	0.47
1:I:831:G:H5''	9:T:37:GLY:HA2	1.95	0.47
3:K:171:TYR:HB3	3:K:183:LYS:HD2	1.97	0.47
8:S:24:VAL:HG13	8:S:33:ALA:HB2	1.97	0.47
11:V:29:VAL:HG12	11:V:29:VAL:O	2.14	0.47
30:C:214:C:H2'	30:C:215:C:C6	2.49	0.47
1:I:723:C:H2'	1:I:724:U:O4'	2.14	0.47
1:I:751:A:C4	52:z:16:AG2:HD2	2.49	0.47
1:I:1169:A:H3'	1:I:1170:C:H5''	1.95	0.47
1:I:2025:C:H2'	1:I:2026:U:C6	2.50	0.47
1:I:2327:A:H3'	1:I:2328:A:C8	2.50	0.47
12:W:34:HIS:HA	12:W:53:THR:OG1	2.13	0.47
29:n:10:G:N3	29:n:10:G:H2'	2.29	0.47
29:n:20:G:H3'	29:n:21:U:H5	1.80	0.47
30:C:1002:G:C6	30:C:1039:G:C6	3.03	0.47
41:q:76:GLU:O	41:q:77:HIS:HB2	2.15	0.47
1:I:1858:A:H2'	1:I:1859:U:O4'	2.15	0.47
1:I:2019:A:H4'	14:Y:34:VAL:HG21	1.96	0.47
1:I:2149:U:H2'	1:I:2150:C:O4'	2.14	0.47
1:I:2183:A:H2'	1:I:2184:A:C8	2.49	0.47
1:I:2788:C:H2'	1:I:2789:C:C6	2.50	0.47
1:I:2800:A:C2	1:I:2895:G:H1'	2.49	0.47
4:L:19:GLY:HA2	13:X:79:PRO:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:123:ARG:HG2	9:T:143:GLU:HB2	1.97	0.47
13:X:91:ALA:HB3	13:X:111:LYS:HG3	1.97	0.47
15:Z:52:PRO:O	15:Z:53:PHE:HB2	2.15	0.47
27:l:27:ALA:O	27:l:28:ASN:HB2	2.14	0.47
29:n:14:A:C2	29:n:15:G:H1'	2.49	0.47
29:n:15:G:C8	29:n:15:G:H5''	2.50	0.47
30:C:203:G:H2'	30:C:204:G:C8	2.50	0.47
30:C:453:G:O5'	30:C:453:G:H8	1.97	0.47
30:C:720:C:H5''	47:w:41:PRO:HA	1.97	0.47
30:C:1225:A:H2'	30:C:1226:C:C5	2.50	0.47
33:F:155:VAL:HG23	33:F:156:LYS:H	1.80	0.47
38:Q:110:GLN:HA	38:Q:110:GLN:OE1	2.14	0.47
52:z:3:ALA:HB1	52:z:10:DAR:HH21	1.79	0.47
1:I:35:G:H2'	1:I:36:G:O4'	2.15	0.47
1:I:611:C:H2'	1:I:612:G:O4'	2.15	0.47
14:Y:24:TYR:HB3	14:Y:28:ARG:HB3	1.96	0.47
30:C:499:A:H4'	30:C:500:G:OP1	2.15	0.47
30:C:850:U:H2'	30:C:851:G:H5''	1.96	0.47
30:C:1005:A:C5	30:C:1006:G:H1'	2.50	0.47
30:C:1035:A:O2'	30:C:1036:A:H5''	2.15	0.47
30:C:1453:G:H5''	30:C:1453:G:N3	2.30	0.47
33:F:173:VAL:HG22	33:F:180:GLY:HA3	1.97	0.47
1:I:2024:G:H2'	1:I:2025:C:O4'	2.15	0.47
1:I:2287:A:H1'	1:I:2288:A:H2'	1.96	0.47
30:C:479:U:O4	56:C:1688:SPD:H22	2.15	0.47
30:C:1002:G:H2'	30:C:1003:G:O4'	2.15	0.47
33:F:124:MET:HB3	33:F:129:VAL:HG22	1.97	0.47
47:w:41:PRO:HB2	47:w:43:ARG:HG2	1.95	0.47
1:I:1868:C:H2'	1:I:1869:G:O4'	2.14	0.47
5:M:79:ARG:HG2	5:M:80:SER:N	2.29	0.47
29:n:2:G:H2'	29:n:3:C:C6	2.49	0.47
29:n:14:A:H2'	29:n:15:G:O4'	2.15	0.47
29:n:50:G:H2'	29:n:51:U:H6	1.76	0.47
30:C:419:C:H5''	30:C:513:C:H4'	1.97	0.47
30:C:436:C:C3'	33:F:153:SER:HB2	2.45	0.47
30:C:594:U:H2'	30:C:595:A:O4'	2.14	0.47
30:C:673:A:H2'	30:C:674:G:C8	2.50	0.47
30:C:757:U:OP1	30:C:822:U:O2'	2.33	0.47
30:C:1135:U:O2'	30:C:1136:C:H2'	2.14	0.47
30:C:1288:A:H2'	30:C:1289:A:O4'	2.14	0.47
30:C:1481:U:H2'	30:C:1482:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1394:U:H4'	1:I:1603:A:H4'	1.95	0.46
23:h:12:SER:O	23:h:16:ARG:NH2	2.49	0.46
30:C:15:G:H21	34:G:23:LYS:HA	1.80	0.46
39:o:9:ARG:HB2	39:o:99:GLN:HB3	1.97	0.46
1:I:1141:U:H4'	1:I:1142:A:O4'	2.14	0.46
30:C:976:G:OP2	30:C:1358:U:O2'	2.33	0.46
41:q:43:LYS:O	41:q:44:LYS:C	2.57	0.46
1:I:1021:A:H3'	1:I:1022:G:H5''	1.96	0.46
1:I:1386:C:H2'	1:I:1387:A:C8	2.50	0.46
10:U:41:LEU:HG	10:U:96:ILE:HG13	1.97	0.46
36:N:146:GLU:HA	36:N:149:LYS:HE2	1.96	0.46
1:I:1794:A:H2'	1:I:1795:C:C6	2.49	0.46
1:I:2578:G:H4'	1:I:2578:G:OP2	2.15	0.46
24:i:25:VAL:O	24:i:26:THR:HB	2.15	0.46
30:C:692:U:H1'	30:C:695:A:N7	2.30	0.46
30:C:1064:G:O2'	30:C:1190:G:N2	2.49	0.46
34:G:79:GLY:O	34:G:120:VAL:HA	2.15	0.46
1:I:2171:A:O2'	1:I:2172:U:H5'	2.16	0.46
30:C:544:G:H5'	30:C:545:C:OP2	2.14	0.46
30:C:1007:U:H2'	30:C:1008:U:C6	2.51	0.46
33:F:138:SER:HB2	33:F:139:PRO:HD2	1.98	0.46
38:Q:11:ARG:HB3	38:Q:106:ARG:HH21	1.79	0.46
39:o:52:LEU:HA	39:o:62:ARG:HG2	1.96	0.46
1:I:2756:U:OP2	28:m:19:ARG:HG2	2.16	0.46
29:n:59:A:O3'	29:n:61:U:H5	1.99	0.46
30:C:408:A:O2'	30:C:409:U:C5'	2.64	0.46
30:C:476:U:H2'	30:C:477:C:C6	2.51	0.46
32:E:25:ASN:O	32:E:29:PHE:HB2	2.16	0.46
33:F:29:ASP:HB3	33:F:33:LYS:N	2.30	0.46
33:F:150:LYS:O	33:F:151:LYS:C	2.57	0.46
33:F:157:ALA:HA	33:F:159:LEU:HD23	1.98	0.46
41:q:4:VAL:HG23	46:v:34:TYR:HB3	1.98	0.46
51:6:25:A:H5'	51:6:25:A:H8	1.81	0.46
1:I:1469:A:H2'	1:I:1470:A:C8	2.50	0.46
1:I:1676:A:H2'	1:I:1677:A:O4'	2.16	0.46
2:J:89:U:O2'	2:J:90:C:H5'	2.16	0.46
5:M:145:ASP:HA	5:M:166:LYS:O	2.15	0.46
9:T:68:SER:O	9:T:69:ARG:HB2	2.15	0.46
29:n:57:C:H2'	29:n:58:A:C8	2.51	0.46
30:C:203:G:O5'	30:C:203:G:H8	1.97	0.46
30:C:216:U:H2'	30:C:217:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:713:G:H2'	30:C:714:G:C8	2.51	0.46
48:x:34:TRP:HA	48:x:52:HIS:HB2	1.98	0.46
1:I:130:C:H2'	1:I:131:A:H5''	1.98	0.46
1:I:1070:A:H3'	1:I:1071:G:H5''	1.97	0.46
1:I:1075:C:H2'	1:I:1076:C:C6	2.51	0.46
6:O:164:TYR:HB2	6:O:167:GLU:HB2	1.98	0.46
29:n:58:A:H2'	29:n:59:A:H5'	1.97	0.46
37:P:105:SER:HB2	37:P:126:ILE:HD11	1.97	0.46
52:z:8:DVA:O	52:z:11:VAL:HG22	2.16	0.46
1:I:185:G:H2'	1:I:186:G:O4'	2.15	0.46
1:I:2570:G:H2'	1:I:2571:U:O4'	2.16	0.46
29:n:62:C:H2'	29:n:63:C:C6	2.51	0.46
30:C:1269:A:C2	30:C:1313:U:O4'	2.69	0.46
47:w:21:ILE:O	47:w:22:ASP:HB3	2.16	0.46
1:I:246:C:C2'	1:I:247:G:H5'	2.46	0.46
1:I:284:U:H2'	1:I:285:G:O5'	2.15	0.46
1:I:2557:G:H2'	1:I:2558:C:C6	2.51	0.46
4:L:25:THR:HG21	4:L:193:VAL:HG22	1.98	0.46
10:U:20:LEU:HD13	19:d:81:PRO:HG2	1.98	0.46
10:U:135:VAL:O	10:U:136:MET:HB3	2.16	0.46
29:n:30:G:H1	29:n:42:C:H42	1.64	0.46
30:C:1021:A:H2'	30:C:1022:A:O4'	2.15	0.46
30:C:1036:A:H2'	30:C:1037:C:C6	2.50	0.46
33:F:157:ALA:C	33:F:159:LEU:H	2.24	0.46
37:P:11:LEU:HD22	37:P:75:ILE:HD11	1.98	0.46
1:I:279:A:H2'	1:I:280:U:O4'	2.16	0.45
1:I:962:G:O2'	1:I:2250:G:N2	2.50	0.45
1:I:2450:A:O2'	29:n:77:A:C2	2.62	0.45
1:I:2467:C:H2'	1:I:2468:A:O4'	2.15	0.45
4:L:172:VAL:HG23	4:L:194:PRO:HD3	1.99	0.45
5:M:159:LEU:HA	5:M:162:ARG:HD3	1.97	0.45
30:C:86:G:H1'	30:C:87:C:C6	2.51	0.45
30:C:1103:C:H5''	31:D:97:LEU:HD22	1.98	0.45
30:C:1274:A:C2'	30:C:1275:A:H5''	2.46	0.45
1:I:839:U:H2'	1:I:840:C:C6	2.52	0.45
1:I:2290:G:H2'	1:I:2291:U:O4'	2.16	0.45
21:f:32:ASN:O	21:f:52:SER:HA	2.17	0.45
29:n:5:G:H2'	29:n:6:G:H8	1.80	0.45
29:n:51:U:H6	29:n:51:U:O5'	1.99	0.45
30:C:757:U:H2'	30:C:758:C:O4'	2.15	0.45
30:C:1486:G:H2'	30:C:1487:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:49:SER:O	42:r:53:ILE:HG12	2.17	0.45
50:5:40:LYS:HG2	50:5:41:PRO:HD2	1.98	0.45
1:I:251:A:C5	1:I:252:G:H1'	2.52	0.45
1:I:460:A:H2'	1:I:461:C:O4'	2.16	0.45
1:I:856:G:H2'	1:I:857:G:C8	2.51	0.45
1:I:1090:A:H2'	1:I:1091:G:C8	2.51	0.45
1:I:1641:A:H2'	1:I:1642:G:O4'	2.16	0.45
1:I:1817:G:C2'	1:I:1818:U:H5'	2.46	0.45
16:a:74:ILE:O	16:a:74:ILE:HG23	2.17	0.45
19:d:70:ILE:HG22	19:d:72:VAL:HG13	1.97	0.45
30:C:51:A:N7	30:C:114:U:O2'	2.47	0.45
30:C:857:C:H2'	30:C:858:G:O4'	2.16	0.45
30:C:1009:U:O2	30:C:1009:U:H2'	2.17	0.45
30:C:1035:A:O2'	30:C:1036:A:C5'	2.65	0.45
30:C:1071:C:H2'	30:C:1072:G:C8	2.51	0.45
30:C:1217:C:OP1	43:s:9:ARG:NE	2.48	0.45
30:C:1218:C:H2'	30:C:1219:A:C8	2.51	0.45
30:C:1307:U:H2'	30:C:1308:U:C6	2.51	0.45
34:G:81:LEU:HB2	34:G:98:PRO:HG3	1.97	0.45
37:P:101:ILE:O	37:P:101:ILE:HG13	2.16	0.45
1:I:646:U:H3'	1:I:647:G:C5'	2.46	0.45
1:I:1735:A:H2'	1:I:1736:U:O4'	2.16	0.45
7:R:110:PRO:O	7:R:115:GLY:HA3	2.16	0.45
30:C:1297:G:N2	36:N:114:LYS:HB3	2.32	0.45
33:F:27:ALA:O	33:F:29:ASP:N	2.50	0.45
49:y:39:ILE:HD13	49:y:82:GLN:HB2	1.98	0.45
2:J:34:A:H5'	2:J:35:C:OP1	2.17	0.45
3:K:205:LEU:HB3	3:K:210:ALA:HB3	1.98	0.45
29:n:49:C:H2'	29:n:60:A:C1'	2.45	0.45
30:C:859:G:H2'	30:C:860:A:C8	2.51	0.45
32:E:55:ILE:HG23	32:E:66:VAL:HG13	1.98	0.45
36:N:88:PRO:HG3	36:N:149:LYS:HA	1.98	0.45
41:q:31:ARG:HE	41:q:58:THR:CG2	2.29	0.45
1:I:1744:A:H3'	1:I:1745:A:C8	2.51	0.45
30:C:418:C:H4'	30:C:419:C:O5'	2.15	0.45
30:C:539:A:N3	30:C:539:A:H5''	2.32	0.45
30:C:1030:U:H5'	30:C:1031:C:H5''	1.98	0.45
30:C:1205:U:H2'	30:C:1206:G:C8	2.51	0.45
1:I:1093:G:H2'	1:I:1094:U:C6	2.52	0.45
1:I:1169:A:C3'	1:I:1170:C:H5''	2.47	0.45
1:I:1669:A:N3	1:I:1669:A:H2'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2016:U:H2'	1:I:2017:U:C6	2.52	0.45
8:S:43:ILE:CD1	8:S:52:VAL:HB	2.47	0.45
15:Z:29:THR:O	15:Z:63:VAL:HB	2.16	0.45
30:C:399:G:H2'	30:C:400:C:C6	2.51	0.45
33:F:13:ARG:CG	33:F:32:CYS:SG	3.05	0.45
33:F:27:ALA:O	33:F:28:ILE:C	2.60	0.45
36:N:70:ARG:HG2	36:N:96:ARG:HB3	1.99	0.45
8:S:24:VAL:HG12	8:S:30:ARG:CD	2.47	0.45
18:c:13:VAL:HG11	18:c:18:ASP:OD1	2.17	0.45
27:l:26:HIS:NE2	27:l:48:ALA:HB2	2.32	0.45
30:C:36:C:O2'	30:C:501:C:H5''	2.17	0.45
30:C:51:A:H4'	30:C:52:C:H5'	1.98	0.45
30:C:115:G:O3'	30:C:116:A:H8	1.99	0.45
30:C:237:G:H5''	46:v:27:ARG:CZ	2.47	0.45
30:C:429:U:OP2	33:F:32:CYS:HB2	2.17	0.45
30:C:1273:C:H2'	30:C:1274:A:O4'	2.17	0.45
1:I:84:A:O2'	18:c:7:ARG:NH2	2.48	0.45
1:I:2591:C:H2'	1:I:2592:G:C8	2.52	0.45
1:I:2646:C:H2'	1:I:2647:U:O4'	2.17	0.45
1:I:2822:G:H2'	1:I:2823:A:H5''	1.98	0.45
30:C:195:A:H2'	30:C:196:A:C8	2.52	0.45
30:C:486:U:H2'	30:C:487:A:C8	2.52	0.45
30:C:492:C:H2'	30:C:493:A:C8	2.52	0.45
30:C:695:A:H5''	30:C:695:A:H8	1.81	0.45
30:C:1193:G:O6	32:E:2:GLY:N	2.50	0.45
32:E:7:PRO:HD2	32:E:184:TYR:CD2	2.52	0.45
35:H:46:GLN:HA	35:H:56:LYS:HG2	1.99	0.45
36:N:97:ASN:OD1	36:N:97:ASN:N	2.49	0.45
39:o:86:ALA:HA	39:o:89:ARG:HE	1.81	0.45
40:p:117:PRO:HD2	50:5:35:ARG:HD2	1.98	0.45
41:q:39:THR:HA	41:q:50:ARG:O	2.17	0.45
1:I:1324:G:H1'	1:I:1616:A:N6	2.32	0.45
1:I:1474:U:H2'	1:I:1475:G:O4'	2.17	0.45
1:I:2497:A:N3	1:I:2498:OMC:N4	2.65	0.45
1:I:2639:A:H2'	1:I:2640:G:O4'	2.17	0.45
3:K:132:MET:HE2	3:K:188:CYS:HB2	1.99	0.45
8:S:40:LYS:HE2	8:S:57:VAL:HG12	1.99	0.45
12:W:90:VAL:O	12:W:117:PHE:HB3	2.17	0.45
30:C:458:U:N3	30:C:459:A:N7	2.65	0.45
30:C:1414:U:H2'	30:C:1415:G:H8	1.81	0.45
31:D:187:VAL:HG11	31:D:193:PRO:HB3	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:F:7:PRO:HB2	33:F:10:LYS:HG3	1.99	0.45
40:p:67:ALA:HB2	40:p:96:THR:HG23	1.99	0.45
1:I:249:C:O2	27:l:12:LYS:NZ	2.45	0.44
1:I:1070:A:H3'	1:I:1071:G:C5'	2.47	0.44
8:S:35:VAL:O	8:S:62:VAL:HB	2.18	0.44
30:C:310:G:H5''	45:u:31:ARG:HB2	1.99	0.44
30:C:1008:U:H3'	30:C:1009:U:H6	1.82	0.44
33:F:122:ALA:O	33:F:145:ILE:HG23	2.17	0.44
38:Q:65:ILE:HD13	38:Q:79:ILE:HG23	1.99	0.44
39:o:65:TYR:HB3	43:s:96:LEU:CD1	2.47	0.44
1:I:657:U:H2'	1:I:658:U:C6	2.52	0.44
1:I:2031:A:C6	1:I:2498:OMC:H1'	2.52	0.44
1:I:2641:G:H5''	7:R:78:THR:HB	1.99	0.44
3:K:155:ALA:HB2	3:K:162:VAL:HG23	2.00	0.44
27:l:45:ARG:H	27:l:46:PRO:HD2	1.81	0.44
30:C:70:U:H1'	30:C:71:A:N7	2.33	0.44
30:C:408:A:O2'	30:C:409:U:H5''	2.17	0.44
30:C:909:A:H2'	30:C:910:C:O4'	2.17	0.44
31:D:26:LYS:HD2	31:D:192:ASP:OD1	2.17	0.44
32:E:6:HIS:CG	43:s:89:MET:HB3	2.52	0.44
33:F:23:SER:HB3	33:F:161:LEU:HD13	1.99	0.44
33:F:145:ILE:HG22	33:F:149:ALA:HB2	1.99	0.44
1:I:45:G:C5'	1:I:46:G:H5'	2.47	0.44
1:I:1908:C:O2'	29:n:12:G:H5''	2.18	0.44
1:I:1965:C:H5''	1:I:1966:A:H2'	1.99	0.44
1:I:2324:U:H3'	1:I:2325:G:C5'	2.48	0.44
1:I:2386:A:H4'	20:e:56:ASP:HA	1.98	0.44
3:K:232:HIS:HA	3:K:242:LYS:CD	2.47	0.44
5:M:58:LYS:HG3	5:M:71:GLY:HA2	1.99	0.44
19:d:28:ALA:HB3	19:d:40:ILE:HG13	1.98	0.44
30:C:545:C:H5'	33:F:69:GLU:CB	2.47	0.44
30:C:1020:G:H2'	30:C:1021:A:C8	2.52	0.44
30:C:1039:G:N3	30:C:1039:G:H2'	2.31	0.44
32:E:77:ILE:HA	32:E:84:VAL:HG13	1.98	0.44
1:I:279:A:OP2	1:I:361:G:N2	2.50	0.44
1:I:479:A:H4'	1:I:480:A:OP1	2.18	0.44
1:I:2111:U:H5	1:I:2145:C:H1'	1.82	0.44
7:R:38:GLY:HA3	7:R:50:THR:HG23	1.99	0.44
24:i:54:VAL:O	24:i:55:ILE:HB	2.18	0.44
29:n:9:G:H4'	29:n:10:G:OP1	2.17	0.44
29:n:13:C:H2'	29:n:13:C:O2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:n:75:C:H2'	29:n:76:C:C6	2.52	0.44
30:C:337:G:H2'	30:C:338:A:C8	2.52	0.44
30:C:1287:A:H2'	30:C:1288:A:C8	2.52	0.44
30:C:1338:G:H2'	30:C:1339:A:C8	2.51	0.44
38:Q:106:ARG:HH11	38:Q:108:ALA:HA	1.82	0.44
39:o:56:HIS:O	39:o:57:VAL:HG22	2.17	0.44
1:I:632:A:H2'	1:I:633:A:C8	2.52	0.44
1:I:716:A:OP1	44:t:88:ARG:NH1	2.50	0.44
1:I:1073:A:H2'	1:I:1074:G:O4'	2.17	0.44
1:I:1746:A:H2'	1:I:1747:U:C6	2.52	0.44
18:c:26:LYS:NZ	18:c:26:LYS:HB3	2.33	0.44
18:c:51:ALA:O	18:c:52:LEU:HB2	2.18	0.44
27:l:31:HIS:ND1	27:l:32:ILE:HG13	2.33	0.44
30:C:109:A:C6	30:C:326:G:C6	3.06	0.44
30:C:435:A:H2'	30:C:436:C:C6	2.53	0.44
30:C:614:C:H2'	30:C:614:C:O2	2.18	0.44
45:u:79:ASN:O	45:u:80:LYS:HB3	2.17	0.44
1:I:468:G:H5''	5:M:55:SER:HB3	1.99	0.44
1:I:1180:U:H2'	1:I:1181:U:O4'	2.17	0.44
1:I:1199:U:H1'	14:Y:4:VAL:HG22	2.00	0.44
1:I:2602:A:H2'	1:I:2602:A:N3	2.32	0.44
1:I:2615:U:C2	24:i:4:GLN:HA	2.53	0.44
10:U:38:ARG:HB2	10:U:98:PRO:HD3	1.99	0.44
13:X:30:VAL:O	13:X:40:LEU:HA	2.18	0.44
23:h:7:ILE:O	23:h:35:THR:HA	2.17	0.44
29:n:6:G:H1	29:n:68:C:H42	1.66	0.44
30:C:250:A:N3	30:C:250:A:H5'	2.33	0.44
30:C:620:C:H1'	33:F:132:ILE:HG21	2.00	0.44
30:C:1274:A:H2'	30:C:1275:A:H5''	2.00	0.44
30:C:1317:C:O5'	43:s:24:ARG:NH2	2.50	0.44
33:F:108:GLY:O	33:F:110:THR:HG23	2.17	0.44
1:I:400:G:N7	21:f:57:ARG:NH2	2.60	0.44
1:I:609:A:H2'	1:I:610:C:O4'	2.18	0.44
1:I:811:U:H2'	9:T:21:ARG:HA	1.99	0.44
1:I:1417:C:H2'	1:I:1418:G:O4'	2.17	0.44
30:C:143:A:H5'	30:C:144:G:H5'	1.99	0.44
30:C:607:A:H2'	30:C:608:A:C8	2.53	0.44
30:C:1101:A:N7	31:D:171:ILE:HG23	2.32	0.44
33:F:124:MET:HA	33:F:129:VAL:HA	1.98	0.44
34:G:77:ASN:O	34:G:80:THR:HG22	2.18	0.44
38:Q:27:LYS:NZ	38:Q:27:LYS:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:534:U:HO2'	14:Y:49:ASP:CG	2.26	0.44
1:I:553:G:H2'	1:I:554:U:O4'	2.18	0.44
1:I:959:A:H2'	1:I:960:A:C8	2.52	0.44
1:I:1081:U:H2'	1:I:1082:U:C6	2.53	0.44
1:I:1642:G:H2'	1:I:1643:G:O4'	2.18	0.44
1:I:2233:U:H2'	1:I:2234:G:C8	2.53	0.44
6:O:85:LYS:HB3	6:O:133:LEU:HD12	1.98	0.44
8:S:15:GLY:HA3	8:S:50:GLY:HA3	2.00	0.44
16:a:63:GLY:O	16:a:64:ALA:HB2	2.18	0.44
30:C:142:G:H3'	30:C:143:A:H8	1.83	0.44
33:F:30:THR:HB	33:F:31:LYS:HE3	1.99	0.44
52:z:6:DVA:HG23	52:z:9:RXL:CA	2.48	0.44
1:I:1028:A:N6	1:I:1125:G:H2'	2.32	0.44
1:I:1703:G:H2'	1:I:1704:C:C6	2.52	0.44
3:K:6:CYS:HB2	3:K:16:VAL:HG23	1.99	0.44
31:D:71:GLY:HA3	31:D:80:VAL:HG21	1.99	0.44
33:F:128:ARG:H	33:F:128:ARG:HD2	1.82	0.44
1:I:84:A:H4'	1:I:85:G:O5'	2.18	0.43
1:I:747:5MU:H72	1:I:2612:C:H4'	1.99	0.43
1:I:2328:A:H2'	1:I:2329:U:C6	2.52	0.43
30:C:429:U:H5''	30:C:430:A:H8	1.83	0.43
30:C:993:G:H2'	30:C:993:G:N3	2.33	0.43
30:C:1367:C:H5'	39:o:62:ARG:NH1	2.33	0.43
31:D:130:THR:O	31:D:131:LYS:HB3	2.18	0.43
1:I:244:A:H2'	1:I:245:G:O4'	2.18	0.43
3:K:226:ASN:C	3:K:233:GLY:HA2	2.43	0.43
10:U:66:ARG:NH1	10:U:104:GLU:OE2	2.51	0.43
30:C:435:A:OP1	30:C:435:A:H4'	2.17	0.43
30:C:947:G:O2'	30:C:1306:A:O2'	2.24	0.43
30:C:1032:G:H3'	30:C:1033:G:H4'	1.99	0.43
30:C:1209:C:H2'	30:C:1210:C:C6	2.54	0.43
41:q:100:GLY:HA3	41:q:118:GLY:HA3	2.00	0.43
1:I:528:A:C2	1:I:2043:C:H4'	2.53	0.43
1:I:1394:U:H2'	1:I:1395:A:O4'	2.17	0.43
1:I:2267:A:H5''	1:I:2268:A:H5'	2.00	0.43
15:Z:52:PRO:O	15:Z:53:PHE:CB	2.67	0.43
29:n:53:G:H1	29:n:63:C:N4	2.16	0.43
30:C:1324:A:O4'	30:C:1362:A:H4'	2.18	0.43
30:C:1346:A:N1	30:C:1374:A:H5''	2.33	0.43
32:E:20:SER:HB3	43:s:94:PRO:HG3	2.00	0.43
36:N:111:ARG:HD2	36:N:123:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:964:C:O2'	1:I:2273:A:N3	2.45	0.43
1:I:2063:C:O2'	29:n:77:A:O2'	2.21	0.43
9:T:77:ILE:HG12	9:T:95:LEU:HD22	2.01	0.43
11:V:29:VAL:HG11	11:V:79:LEU:HG	1.99	0.43
22:g:4:LYS:HB2	22:g:4:LYS:HE2	1.92	0.43
30:C:81:A:N3	30:C:81:A:H2'	2.32	0.43
30:C:160:A:H2'	30:C:161:A:O4'	2.18	0.43
30:C:436:C:H4'	33:F:153:SER:CB	2.48	0.43
30:C:462:G:H2'	30:C:463:U:C6	2.54	0.43
30:C:1021:A:H2'	30:C:1022:A:C1'	2.49	0.43
30:C:1032:G:C3'	30:C:1033:G:H4'	2.48	0.43
30:C:1305:G:C2	30:C:1331:G:N3	2.86	0.43
31:D:67:ILE:HD12	31:D:160:ALA:HB3	2.01	0.43
47:w:32:TYR:HB3	47:w:55:LEU:HD21	2.00	0.43
1:I:565:C:H2'	1:I:566:U:O4'	2.17	0.43
1:I:1348:C:H2'	1:I:1349:C:H5'	1.99	0.43
1:I:2619:C:H5''	4:L:157:LYS:HA	2.00	0.43
8:S:35:VAL:HG22	8:S:69:VAL:HG22	2.00	0.43
13:X:18:PRO:HG3	13:X:84:ILE:O	2.19	0.43
13:X:39:ARG:NH2	30:C:346:G:OP1	2.52	0.43
16:a:31:GLN:O	16:a:35:ILE:HG13	2.19	0.43
29:n:8:U:H6	29:n:8:U:O5'	2.02	0.43
29:n:49:C:C2'	29:n:60:A:H1'	2.47	0.43
30:C:131:A:H2'	30:C:132:C:C6	2.54	0.43
30:C:135:C:OP1	56:C:1689:SPD:H41	2.18	0.43
30:C:555:U:H2'	30:C:556:C:C6	2.54	0.43
30:C:1033:G:H2'	30:C:1034:G:C1'	2.48	0.43
30:C:1261:A:N3	30:C:1261:A:H2'	2.33	0.43
30:C:1527:U:H2'	30:C:1528:U:C6	2.54	0.43
33:F:11:LEU:HB3	33:F:63:ARG:HD3	2.00	0.43
46:v:10:GLY:HA3	46:v:25:ILE:HD13	2.00	0.43
1:I:567:U:H2'	1:I:568:U:O4'	2.19	0.43
1:I:608:A:H2'	1:I:609:A:C8	2.53	0.43
1:I:717:C:H3'	1:I:718:A:H8	1.84	0.43
1:I:1384:A:H1'	1:I:1405:U:H1'	2.01	0.43
1:I:1736:U:H2'	1:I:1737:G:O4'	2.18	0.43
1:I:2012:G:N7	16:a:16:LYS:NZ	2.65	0.43
1:I:2537:U:H2'	1:I:2538:C:C6	2.54	0.43
6:O:89:LEU:HB3	6:O:94:TYR:HB3	2.01	0.43
16:a:84:ARG:O	16:a:95:ARG:HA	2.19	0.43
17:b:30:ILE:HG13	17:b:30:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:f:11:ARG:HB2	21:f:12:PRO:HD2	1.99	0.43
30:C:87:C:H2'	30:C:88:U:C6	2.53	0.43
30:C:382:A:H2'	30:C:383:A:C8	2.53	0.43
30:C:418:C:H5'	30:C:419:C:C5	2.54	0.43
30:C:613:C:O2	30:C:613:C:H2'	2.18	0.43
30:C:1463:U:H2'	30:C:1464:U:C6	2.53	0.43
35:H:3:HIS:HB3	35:H:92:THR:OG1	2.19	0.43
43:s:89:MET:HE2	43:s:89:MET:HA	2.01	0.43
46:v:21:ILE:HG12	46:v:48:ASP:HB2	2.01	0.43
1:I:2140:G:H3'	1:I:2141:G:H8	1.83	0.43
1:I:2445:2MG:HM21	1:I:2449:U:O4	2.19	0.43
1:I:2451:A:H5''	1:I:2451:A:H8	1.83	0.43
1:I:2804:U:H2'	1:I:2805:C:C6	2.53	0.43
30:C:6:G:O2'	30:C:7:A:H8	2.01	0.43
30:C:427:U:H4'	30:C:542:G:OP1	2.19	0.43
30:C:436:C:H4'	33:F:153:SER:HB2	2.01	0.43
30:C:640:A:H2'	30:C:641:U:O4'	2.18	0.43
30:C:913:A:H1'	30:C:914:A:H1'	2.00	0.43
39:o:53:ILE:HD11	39:o:61:ALA:HB1	2.00	0.43
1:I:1723:G:H2'	1:I:1724:G:O4'	2.18	0.43
1:I:2026:U:H2'	1:I:2027:G:O4'	2.18	0.43
1:I:2168:G:H2'	1:I:2169:A:C8	2.54	0.43
1:I:2825:G:H5''	1:I:2825:G:N3	2.34	0.43
5:M:35:TYR:CE2	5:M:176:ASP:HB2	2.54	0.43
22:g:36:GLN:O	22:g:37:LEU:C	2.61	0.43
30:C:294:U:H2'	30:C:295:C:C6	2.54	0.43
30:C:364:A:H2'	30:C:365:U:O2	2.19	0.43
30:C:434:U:O2'	30:C:435:A:P	2.76	0.43
30:C:608:A:H2'	30:C:609:A:O4'	2.18	0.43
30:C:994:A:N3	30:C:994:A:H2'	2.33	0.43
30:C:1053:G:H4'	30:C:1054:C:H3'	2.01	0.43
33:F:105:MET:CG	33:F:173:VAL:HG21	2.48	0.43
33:F:110:THR:O	33:F:111:ARG:HB3	2.19	0.43
37:P:53:GLY:HA3	37:P:57:PRO:HA	2.00	0.43
1:I:1283:G:H1'	1:I:1329:U:O2	2.19	0.43
1:I:1744:A:H3'	1:I:1745:A:H8	1.84	0.43
1:I:1783:A:H5'	1:I:2608:G:H4'	2.01	0.43
1:I:2286:G:H4'	1:I:2287:A:O4'	2.19	0.43
5:M:45:ALA:HB2	5:M:89:PRO:HD3	2.01	0.43
14:Y:24:TYR:HB3	14:Y:28:ARG:CB	2.49	0.43
32:E:10:ILE:HG23	32:E:11:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:F:165:ARG:HD2	33:F:165:ARG:N	2.34	0.43
33:F:202:GLU:OE1	34:G:112:ARG:NH1	2.52	0.43
1:I:2514:U:H2'	1:I:2515:C:C6	2.53	0.43
3:K:153:GLN:HA	3:K:156:ARG:HD3	2.01	0.43
9:T:64:PHE:HB3	27:l:25:LYS:HD2	2.00	0.43
22:g:26:PHE:O	22:g:29:ARG:HG2	2.19	0.43
29:n:68:C:O2	29:n:68:C:C2'	2.66	0.43
30:C:524:G:H2'	30:C:525:C:C6	2.54	0.43
30:C:848:C:H2'	30:C:849:G:O4'	2.19	0.43
30:C:997:U:H2'	30:C:998:C:C6	2.54	0.43
31:D:49:MET:O	31:D:52:GLU:HG2	2.19	0.43
33:F:37:ALA:HB1	33:F:38:PRO:HD2	2.00	0.43
1:I:547:A:N3	1:I:547:A:H2'	2.34	0.42
1:I:1068:G:H2'	1:I:1096:A:O2'	2.18	0.42
1:I:1186:G:H2'	1:I:1187:G:O4'	2.19	0.42
1:I:2074:U:H2'	1:I:2075:U:C6	2.54	0.42
1:I:2687:U:H2'	1:I:2688:G:O4'	2.17	0.42
7:R:83:GLY:O	7:R:85:LYS:HG2	2.18	0.42
27:l:45:ARG:N	27:l:46:PRO:HD2	2.34	0.42
30:C:17:U:H2'	30:C:18:C:C6	2.53	0.42
30:C:159:G:H8	30:C:159:G:H5''	1.83	0.42
30:C:517:G:H5'	30:C:519:C:C2	2.54	0.42
30:C:1028:C:H2'	30:C:1029:U:O4'	2.19	0.42
30:C:1041:G:H2'	30:C:1042:A:O4'	2.19	0.42
30:C:1139:G:H5''	30:C:1140:C:H5	1.83	0.42
30:C:1381:U:H2'	30:C:1382:C:O4'	2.19	0.42
43:s:33:ASP:HB3	43:s:36:ALA:HB2	2.00	0.42
1:I:667:U:H2'	1:I:668:A:O4'	2.19	0.42
1:I:1727:C:H2'	1:I:1728:C:O4'	2.18	0.42
5:M:121:VAL:O	5:M:189:THR:HA	2.18	0.42
18:c:74:ASN:O	18:c:75:ALA:HB3	2.18	0.42
30:C:545:C:H5'	33:F:69:GLU:HB2	2.00	0.42
35:H:49:TYR:OH	35:H:86:ARG:NH1	2.48	0.42
37:P:116:ALA:HB1	37:P:121:LEU:O	2.19	0.42
42:r:4:ILE:HD11	42:r:53:ILE:HD12	2.01	0.42
49:y:28:MET:HE1	49:y:67:ILE:HG21	2.01	0.42
1:I:521:U:H2'	1:I:522:A:C8	2.55	0.42
1:I:2297:A:H2'	1:I:2322:A:H1'	2.01	0.42
1:I:2324:U:H3'	1:I:2325:G:H5''	2.01	0.42
1:I:2823:A:OP1	4:L:118:PHE:HB2	2.18	0.42
6:O:35:ARG:NE	6:O:75:MET:SD	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:53:MET:HE1	10:U:103:TYR:CG	2.54	0.42
29:n:42:C:H1'	30:C:1339:A:H1'	2.01	0.42
30:C:149:A:H4'	30:C:149:A:OP1	2.20	0.42
30:C:1289:A:H5''	30:C:1290:G:C8	2.54	0.42
33:F:13:ARG:NH2	33:F:33:LYS:HE2	2.34	0.42
1:I:1341:G:H5'	17:b:61:LEU:HB3	2.02	0.42
1:I:1739:A:H2'	1:I:1740:G:O4'	2.19	0.42
1:I:2636:C:H2'	1:I:2637:U:C6	2.54	0.42
1:I:2849:U:H4'	1:I:2868:A:C2	2.55	0.42
2:J:116:G:H2'	2:J:117:G:O4'	2.19	0.42
24:i:38:HIS:HB3	24:i:44:THR:HG22	2.01	0.42
27:l:8:ARG:HE	27:l:8:ARG:HA	1.84	0.42
29:n:12:G:C2	29:n:13:C:H1'	2.55	0.42
30:C:179:A:H2'	30:C:180:U:O4'	2.18	0.42
33:F:188:ARG:HB3	33:F:188:ARG:HH11	1.85	0.42
42:r:16:VAL:O	42:r:20:THR:HG23	2.19	0.42
1:I:250:G:H4'	9:T:59:ARG:HD2	2.00	0.42
1:I:2852:G:H2'	1:I:2853:C:O4'	2.20	0.42
9:T:91:ASP:HB2	9:T:94:THR:HG23	2.01	0.42
28:m:4:ARG:O	28:m:37:GLN:HA	2.20	0.42
30:C:76:G:H3'	30:C:77:A:H8	1.84	0.42
30:C:411:A:C2	33:F:31:LYS:HE3	2.54	0.42
30:C:1006:G:H8	30:C:1006:G:OP2	2.03	0.42
30:C:1348:U:O2	30:C:1348:U:H2'	2.20	0.42
33:F:170:TRP:O	33:F:183:LYS:HD3	2.19	0.42
34:G:56:VAL:N	34:G:57:PRO:HD2	2.35	0.42
36:N:140:ASP:OD1	36:N:143:ARG:NH2	2.52	0.42
1:I:974:G:H1'	1:I:975:A:C8	2.54	0.42
1:I:1061:U:O3'	1:I:1070:A:H4'	2.19	0.42
1:I:1354:A:H2'	1:I:1355:G:O4'	2.20	0.42
1:I:1526:C:H2'	1:I:1527:G:O4'	2.19	0.42
1:I:1933:G:H2'	1:I:1934:C:O4'	2.20	0.42
1:I:2395:C:H2'	1:I:2396:G:O4'	2.20	0.42
1:I:2408:U:H2'	1:I:2409:G:C8	2.54	0.42
1:I:2635:A:C2	1:I:2636:C:H1'	2.55	0.42
1:I:2756:U:H1'	1:I:2757:A:H5''	2.00	0.42
8:S:9:ASN:O	8:S:83:ALA:HA	2.19	0.42
8:S:109:SER:O	8:S:110:GLU:HB3	2.20	0.42
15:Z:54:VAL:HG22	15:Z:55:ASP:H	1.85	0.42
16:a:70:LYS:NZ	16:a:70:LYS:CB	2.83	0.42
29:n:19:G:C5	29:n:58:A:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:140:U:H2'	30:C:141:G:O4'	2.19	0.42
30:C:429:U:H4'	30:C:430:A:O5'	2.20	0.42
30:C:619:U:O2'	33:F:130:VAL:HG22	2.19	0.42
30:C:909:A:N3	30:C:1413:A:O2'	2.47	0.42
1:I:362:A:H2'	1:I:362:A:N3	2.35	0.42
1:I:1246:A:H2'	1:I:1247:A:O4'	2.20	0.42
1:I:1568:G:H4'	3:K:59:LYS:HG2	2.01	0.42
1:I:1786:A:H1'	1:I:1938:A:N6	2.35	0.42
1:I:2625:G:H2'	1:I:2626:C:O4'	2.20	0.42
9:T:77:ILE:CD1	9:T:108:ALA:HB1	2.49	0.42
12:W:18:LEU:HD13	12:W:25:ARG:HB3	2.02	0.42
29:n:55:U:H2'	29:n:56:U:O2	2.18	0.42
30:C:967:C:H2'	30:C:968:A:C8	2.55	0.42
30:C:1371:G:O3'	38:Q:71:GLY:HA3	2.20	0.42
32:E:188:GLU:HB3	32:E:195:VAL:HG13	2.01	0.42
33:F:173:VAL:HG13	33:F:179:GLU:O	2.19	0.42
46:v:64:CYS:SG	46:v:74:THR:HG23	2.60	0.42
1:I:231:A:H2'	1:I:232:G:O4'	2.20	0.42
1:I:297:G:H2'	1:I:298:G:O4'	2.20	0.42
1:I:414:C:H2'	1:I:415:A:C8	2.55	0.42
1:I:581:C:H2'	1:I:582:A:C8	2.55	0.42
1:I:621:A:H2'	1:I:622:G:O4'	2.20	0.42
1:I:817:C:H2'	1:I:818:G:O4'	2.20	0.42
1:I:1515:A:H2'	1:I:1516:G:O4'	2.20	0.42
1:I:2086:U:H2'	1:I:2087:G:C8	2.55	0.42
1:I:2298:A:H2'	1:I:2299:U:O4'	2.19	0.42
1:I:2792:A:H2'	1:I:2793:C:O4'	2.20	0.42
4:L:14:ILE:HG12	4:L:24:VAL:HG21	2.01	0.42
8:S:92:GLU:O	8:S:93:GLN:HB2	2.20	0.42
30:C:2:A:H4'	30:C:3:A:H5'	2.02	0.42
35:H:10:VAL:HG12	35:H:11:HIS:N	2.35	0.42
35:H:38:ARG:CG	35:H:40:GLU:HG2	2.50	0.42
1:I:228:C:H4'	1:I:229:C:H5''	2.02	0.42
1:I:729:G:C6	3:K:207:LYS:HB2	2.55	0.42
1:I:1433:A:H2'	1:I:1434:A:O4'	2.20	0.42
1:I:1571:A:H2'	1:I:1572:A:C8	2.55	0.42
1:I:1666:G:O2'	1:I:1667:G:H5'	2.20	0.42
1:I:2690:U:O2'	1:I:2872:A:H1'	2.19	0.42
4:L:85:ALA:O	4:L:86:GLU:HB3	2.20	0.42
22:g:2:LYS:O	22:g:4:LYS:HD3	2.20	0.42
24:i:40:ARG:HG2	24:i:41:HIS:ND1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:2:A:P	30:C:2:A:H2'	2.60	0.42
30:C:292:G:C5	30:C:293:G:H1'	2.55	0.42
30:C:374:A:H2'	30:C:375:U:C6	2.54	0.42
30:C:433:G:H3'	30:C:434:U:H5'	2.02	0.42
30:C:452:A:H5''	30:C:452:A:N3	2.35	0.42
30:C:543:U:H5'	30:C:544:G:OP2	2.20	0.42
30:C:651:C:H2'	30:C:652:U:C6	2.55	0.42
30:C:685:G:H2'	30:C:686:U:C6	2.55	0.42
30:C:766:A:H2'	30:C:767:A:O4'	2.20	0.42
30:C:1036:A:C2	30:C:1037:C:N4	2.88	0.42
30:C:1268:G:O5'	30:C:1268:G:H8	2.03	0.42
40:p:79:ILE:HB	40:p:105:PHE:HE2	1.84	0.42
46:v:17:MET:CB	46:v:20:SER:HB2	2.50	0.42
1:I:278:A:N1	1:I:361:G:H1'	2.35	0.42
1:I:974:G:O2'	1:I:989:G:N2	2.53	0.42
1:I:1580:A:H2'	1:I:1581:G:O4'	2.19	0.42
9:T:142:ILE:HD12	9:T:142:ILE:N	2.35	0.42
15:Z:39:LEU:O	15:Z:40:MET:HB2	2.19	0.42
19:d:26:PHE:CE2	19:d:89:ILE:HD13	2.55	0.42
30:C:8:A:H1'	34:G:108:GLY:HA2	2.02	0.42
30:C:628:G:H2'	30:C:629:A:H8	1.83	0.42
30:C:992:U:O2'	30:C:1043:G:N7	2.50	0.42
30:C:1227:A:H4'	42:r:114:LYS:HE2	2.02	0.42
30:C:1318:A:H4'	48:x:10:PHE:CE2	2.55	0.42
32:E:70:THR:HG21	32:E:76:VAL:HG21	2.01	0.42
33:F:9:LEU:HB3	33:F:32:CYS:SG	2.60	0.42
33:F:107:PHE:CE1	33:F:155:VAL:HB	2.54	0.42
1:I:191:A:H2'	1:I:192:C:C6	2.55	0.41
1:I:1672:A:C2	1:I:2582:G:H5'	2.55	0.41
1:I:2451:A:H5''	1:I:2451:A:C8	2.54	0.41
3:K:16:VAL:HG12	3:K:205:LEU:O	2.19	0.41
6:O:24:ILE:HG12	6:O:26:ILE:HD11	2.02	0.41
16:a:67:ASP:N	16:a:67:ASP:OD1	2.53	0.41
29:n:6:G:H8	29:n:6:G:O5'	2.03	0.41
30:C:89:U:H2'	30:C:90:C:O4'	2.20	0.41
30:C:373:A:H2'	30:C:373:A:N3	2.35	0.41
30:C:431:A:H4'	30:C:432:A:OP1	2.19	0.41
30:C:1330:U:H2'	30:C:1331:G:O4'	2.20	0.41
32:E:130:PHE:CE2	32:E:131:ARG:HG3	2.55	0.41
33:F:57:GLU:HG3	33:F:199:LEU:HD12	2.02	0.41
1:I:289:G:H2'	1:I:290:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:511:U:O4	1:I:512:G:N1	2.52	0.41
1:I:1063:G:H2'	1:I:1064:C:O4'	2.20	0.41
1:I:2146:C:H4'	1:I:2147:A:C8	2.55	0.41
1:I:2251:OMG:HM23	1:I:2251:OMG:H1'	1.69	0.41
3:K:167:ARG:HG3	3:K:172:VAL:HG12	2.02	0.41
28:m:26:ILE:O	28:m:26:ILE:HG13	2.20	0.41
30:C:144:G:H2'	30:C:145:G:C8	2.55	0.41
30:C:266:G:H1'	30:C:268:U:OP2	2.20	0.41
31:D:94:HIS:O	31:D:95:ARG:C	2.62	0.41
33:F:105:MET:CG	33:F:171:LEU:HD13	2.51	0.41
39:o:30:LYS:HA	39:o:34:ALA:O	2.20	0.41
1:I:278:A:N3	1:I:278:A:H2'	2.35	0.41
1:I:396:G:H1'	21:f:29:PHE:HB3	2.01	0.41
1:I:1370:C:H2'	1:I:1371:G:O4'	2.21	0.41
1:I:1507:C:H2'	1:I:1508:A:H4'	2.02	0.41
1:I:2038:G:H2'	1:I:2039:U:O4'	2.20	0.41
30:C:51:A:H4'	30:C:52:C:C5'	2.50	0.41
30:C:718:A:H4'	50:5:34:ARG:HH22	1.85	0.41
30:C:1027:C:H2'	30:C:1028:C:C6	2.55	0.41
32:E:138:VAL:O	32:E:142:MET:HG2	2.20	0.41
33:F:83:LYS:H	33:F:83:LYS:HD2	1.85	0.41
33:F:107:PHE:CD1	33:F:155:VAL:HB	2.56	0.41
39:o:25:ILE:O	39:o:28:THR:HG22	2.20	0.41
42:r:11:ASP:HA	42:r:45:ILE:HB	2.03	0.41
48:x:32:ARG:HA	48:x:50:ALA:HB3	2.02	0.41
1:I:241:A:N1	1:I:255:A:H5''	2.35	0.41
1:I:246:C:H2'	1:I:247:G:H5'	2.01	0.41
1:I:328:U:O3'	18:c:66:GLN:HG3	2.21	0.41
1:I:690:G:H2'	1:I:691:C:O4'	2.20	0.41
1:I:732:C:H2'	1:I:733:G:O4'	2.20	0.41
1:I:1853:A:H2'	1:I:1854:A:C8	2.56	0.41
1:I:2017:U:H4'	24:i:5:GLN:O	2.21	0.41
1:I:2155:U:H2'	1:I:2156:G:O4'	2.19	0.41
2:J:106:G:H2'	2:J:107:G:O4'	2.20	0.41
4:L:121:THR:HB	4:L:127:PHE:CD2	2.56	0.41
6:O:8:PRO:HB3	6:O:51:THR:HA	2.02	0.41
29:n:70:C:H2'	29:n:71:G:C8	2.55	0.41
30:C:452:A:H2'	30:C:453:G:H5'	2.01	0.41
30:C:965:U:H5''	30:C:966:G:OP1	2.20	0.41
30:C:1317:C:O2	30:C:1317:C:H2'	2.20	0.41
32:E:206:GLU:HB3	32:E:207:ILE:H	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:283:G:H2'	1:I:284:U:O4'	2.21	0.41
1:I:858:G:O2'	1:I:2268:A:H1'	2.21	0.41
1:I:1385:A:H1'	1:I:1386:C:C6	2.55	0.41
1:I:1482:G:N2	1:I:1508:A:H1'	2.35	0.41
1:I:1500:G:H2'	1:I:1501:G:O4'	2.21	0.41
1:I:1667:G:H5''	8:S:5:GLN:O	2.21	0.41
1:I:1824:G:O3'	3:K:247:PRO:HD3	2.20	0.41
1:I:2520:C:C6	1:I:2567:G:H1'	2.54	0.41
6:O:156:PRO:O	6:O:171:THR:HA	2.20	0.41
7:R:36:LEU:O	7:R:51:GLY:HA3	2.21	0.41
11:V:33:ILE:HD13	11:V:114:GLU:HB3	2.03	0.41
24:i:40:ARG:HG2	24:i:41:HIS:HD1	1.85	0.41
25:j:4:GLY:O	25:j:5:ILE:HB	2.21	0.41
30:C:1005:A:H5''	30:C:1038:C:H1'	2.03	0.41
30:C:1029:U:O2	30:C:1029:U:H2'	2.21	0.41
30:C:1309:G:N7	42:r:98:ARG:NH2	2.69	0.41
32:E:19:ASN:O	32:E:56:VAL:HA	2.21	0.41
33:F:159:LEU:O	33:F:163:GLU:HG2	2.20	0.41
36:N:71:PRO:O	36:N:96:ARG:HD3	2.20	0.41
41:q:31:ARG:HH12	41:q:33:VAL:HG23	1.84	0.41
1:I:193:U:O3'	1:I:803:U:H4'	2.20	0.41
1:I:354:A:H2'	1:I:355:U:C6	2.55	0.41
1:I:878:A:H3'	1:I:879:G:H8	1.85	0.41
1:I:1570:A:H2'	1:I:1571:A:C8	2.55	0.41
1:I:1738:G:H8	1:I:1738:G:H5''	1.84	0.41
1:I:2182:U:H2'	1:I:2183:A:N7	2.35	0.41
1:I:2514:U:H4'	7:R:81:ILE:HG12	2.03	0.41
13:X:14:LYS:HD3	13:X:77:HIS:HA	2.03	0.41
16:a:25:ARG:NH2	16:a:74:ILE:O	2.51	0.41
30:C:413:G:H21	30:C:428:G:H21	1.68	0.41
30:C:499:A:H1'	30:C:500:G:C8	2.55	0.41
30:C:727:G:N2	30:C:730:G:OP2	2.46	0.41
30:C:994:A:N1	30:C:1047:G:H4'	2.35	0.41
30:C:1394:A:H8	30:C:1394:A:OP1	2.03	0.41
42:r:4:ILE:HD12	42:r:9:ILE:HD11	2.03	0.41
1:I:192:C:H2'	1:I:193:U:H5'	2.02	0.41
1:I:528:A:C2	1:I:2042:A:H2'	2.56	0.41
1:I:613:A:H3'	1:I:614:A:H5'	2.02	0.41
1:I:1104:C:H2'	1:I:1105:U:C6	2.55	0.41
1:I:1418:G:H2'	1:I:1579:A:N6	2.36	0.41
1:I:1584:U:C2'	1:I:1585:C:H5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2063:C:H1'	55:n:101:FME:H	1.85	0.41
1:I:2065:C:H2'	1:I:2066:C:C6	2.56	0.41
3:K:182:ARG:HG3	3:K:267:ILE:HD13	2.03	0.41
3:K:260:ASN:C	3:K:262:ARG:H	2.29	0.41
6:O:54:PRO:HG3	6:O:62:TRP:CE2	2.56	0.41
13:X:111:LYS:HB2	13:X:111:LYS:NZ	2.36	0.41
19:d:7:GLU:HB2	19:d:41:GLU:HG3	2.02	0.41
30:C:537:G:H2'	30:C:538:G:H5''	2.02	0.41
30:C:543:U:O2	30:C:543:U:H2'	2.20	0.41
30:C:1138:G:H3'	30:C:1138:G:N3	2.36	0.41
30:C:1158:C:C5	30:C:1160:G:H1'	2.56	0.41
30:C:1170:A:H2'	30:C:1171:A:O4'	2.21	0.41
1:I:226:A:H2'	1:I:227:A:O4'	2.21	0.41
1:I:337:C:H2'	1:I:338:G:O4'	2.20	0.41
1:I:942:G:H4'	1:I:1190:G:H5'	2.03	0.41
1:I:1327:A:H2'	1:I:1328:A:O4'	2.21	0.41
1:I:1873:G:H2'	1:I:1874:C:C6	2.56	0.41
1:I:2840:C:H5''	11:V:53:THR:OG1	2.20	0.41
13:X:33:VAL:HG22	13:X:38:LYS:HG3	2.01	0.41
16:a:27:LYS:O	16:a:70:LYS:HG3	2.20	0.41
29:n:9:G:N3	29:n:46:G:H2'	2.36	0.41
30:C:404:G:H4'	30:C:439:U:O2	2.21	0.41
30:C:1017:U:H2'	30:C:1018:G:C8	2.56	0.41
30:C:1146:A:H2'	30:C:1146:A:N3	2.34	0.41
33:F:185:LYS:HG3	33:F:186:PRO:HD2	2.02	0.41
33:F:201:VAL:HG11	34:G:102:GLY:O	2.20	0.41
42:r:90:ARG:HD3	42:r:96:PRO:O	2.20	0.41
47:w:47:THR:HG22	47:w:48:ARG:N	2.36	0.41
1:I:285:G:H3'	1:I:286:U:C6	2.56	0.41
1:I:307:G:N2	1:I:309:A:H3'	2.36	0.41
1:I:773:U:O2'	3:K:48:ARG:HD3	2.20	0.41
1:I:832:U:H2'	1:I:833:A:C8	2.56	0.41
1:I:918:A:H5''	2:J:97:C:O2'	2.21	0.41
1:I:1493:C:O2'	1:I:1494:A:H5'	2.21	0.41
1:I:1747:U:H2'	1:I:1748:C:C6	2.56	0.41
1:I:1866:A:H2'	1:I:1867:G:H5'	2.03	0.41
1:I:1993:U:H2'	1:I:1994:C:O4'	2.21	0.41
1:I:2020:A:H5'	24:i:9:THR:CG2	2.51	0.41
1:I:2297:A:N1	1:I:2321:U:H5	2.18	0.41
2:J:34:A:H4'	2:J:35:C:H5'	2.02	0.41
10:U:26:VAL:HG13	10:U:104:GLU:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:58:ARG:HA	14:Y:61:TRP:CE3	2.56	0.41
22:g:2:LYS:O	22:g:3:ALA:HB3	2.21	0.41
30:C:60:A:N1	30:C:107:G:O2'	2.54	0.41
30:C:299:G:O5'	30:C:299:G:H8	2.04	0.41
30:C:436:C:O2	30:C:437:U:C5	2.74	0.41
30:C:461:A:H2'	30:C:462:G:C8	2.56	0.41
30:C:491:G:H2'	30:C:492:C:C6	2.55	0.41
30:C:1206:G:H2'	30:C:1206:G:N3	2.36	0.41
30:C:1298:U:OP2	36:N:114:LYS:HE2	2.21	0.41
30:C:1320:C:H2'	30:C:1321:U:C6	2.56	0.41
30:C:1492:A:H8	30:C:1492:A:H5''	1.86	0.41
33:F:11:LEU:HB3	33:F:19:LEU:CD1	2.51	0.41
33:F:145:ILE:N	33:F:145:ILE:HD12	2.36	0.41
33:F:156:LYS:HG2	33:F:157:ALA:H	1.86	0.41
35:H:29:ILE:HG21	35:H:64:VAL:CG2	2.51	0.41
36:N:132:GLY:O	36:N:135:VAL:HG22	2.20	0.41
38:Q:21:ILE:CG2	38:Q:61:LEU:HD13	2.51	0.41
39:o:8:ILE:O	39:o:74:VAL:HG22	2.21	0.41
39:o:36:VAL:HG21	39:o:74:VAL:HB	2.03	0.41
1:I:284:U:C2'	1:I:285:G:O5'	2.69	0.41
1:I:851:C:H2'	1:I:852:U:C6	2.55	0.41
1:I:1020:A:N1	1:I:1141:U:H1'	2.36	0.41
1:I:1187:G:H5''	15:Z:83:TYR:CE1	2.56	0.41
1:I:1652:A:N6	11:V:11:ASN:OD1	2.54	0.41
1:I:1809:A:H2'	1:I:1810:A:C8	2.56	0.41
1:I:2097:A:H2'	1:I:2098:U:C6	2.55	0.41
2:J:64:G:H2'	2:J:65:U:C6	2.56	0.41
3:K:145:GLU:HG2	3:K:151:GLY:C	2.45	0.41
14:Y:73:GLY:O	14:Y:74:ILE:HB	2.21	0.41
19:d:48:MET:SD	19:d:51:GLN:NE2	2.94	0.41
24:i:44:THR:HG23	24:i:48:TYR:O	2.21	0.41
30:C:6:G:C4	34:G:124:LEU:HD11	2.56	0.41
30:C:424:G:H8	30:C:424:G:OP2	2.03	0.41
30:C:632:U:O2	30:C:632:U:H2'	2.20	0.41
30:C:1219:A:H2'	30:C:1220:G:C8	2.56	0.41
40:p:112:ASP:O	47:w:73:ARG:HD3	2.20	0.41
43:s:32:SER:O	43:s:33:ASP:C	2.63	0.41
44:t:69:TYR:O	44:t:72:ARG:HG2	2.20	0.41
1:I:127:A:H5''	1:I:128:C:O4'	2.21	0.40
1:I:458:G:C8	26:k:37:LYS:HG2	2.56	0.40
1:I:1139:G:O3'	7:R:26:GLY:HA3	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1297:C:O2'	1:I:1302:A:N1	2.53	0.40
57:I:3213:HOH:O	55:n:101:FME:HE3	2.21	0.40
3:K:94:VAL:HG22	3:K:102:ARG:O	2.20	0.40
18:c:44:LYS:HB3	18:c:59:VAL:CG2	2.51	0.40
30:C:113:G:H4'	30:C:355:C:OP1	2.21	0.40
30:C:282:A:N3	30:C:282:A:H2'	2.36	0.40
30:C:355:C:H5''	30:C:389:A:OP2	2.21	0.40
30:C:363:A:OP1	41:q:31:ARG:N	2.48	0.40
30:C:570:G:O2'	30:C:819:A:H5''	2.22	0.40
30:C:621:A:H2'	30:C:622:A:C8	2.56	0.40
1:I:1923:U:H2'	1:I:1924:C:C6	2.56	0.40
1:I:2033:A:H4'	1:I:2034:U:OP1	2.21	0.40
1:I:2160:C:H2'	1:I:2161:C:O4'	2.21	0.40
2:J:39:A:H2'	2:J:40:U:C6	2.56	0.40
2:J:50:A:H2'	2:J:51:G:O4'	2.21	0.40
5:M:48:THR:HG23	5:M:86:ALA:HB3	2.04	0.40
6:O:126:PRO:HD3	6:O:132:VAL:HG22	2.02	0.40
6:O:138:LYS:O	6:O:141:ILE:HG22	2.21	0.40
10:U:78:LEU:O	10:U:79:ALA:HB3	2.22	0.40
29:n:9:G:C4'	29:n:47:G:H1'	2.51	0.40
29:n:17:C:OP1	29:n:61:U:H1'	2.21	0.40
29:n:34:U:C5	38:Q:130:ARG:NE	2.89	0.40
29:n:34:U:C5	38:Q:130:ARG:NH1	2.88	0.40
30:C:236:A:H2'	30:C:237:G:C8	2.56	0.40
30:C:1410:A:H2'	30:C:1411:C:C6	2.57	0.40
32:E:121:THR:HG21	32:E:187:SER:HB3	2.03	0.40
38:Q:32:GLN:HA	38:Q:32:GLN:OE1	2.22	0.40
42:r:33:ILE:HD13	42:r:60:VAL:HG22	2.03	0.40
49:y:20:HIS:O	49:y:24:ARG:HG2	2.21	0.40
1:I:229:C:H2'	1:I:230:G:O4'	2.21	0.40
1:I:582:A:H2'	1:I:583:G:C8	2.56	0.40
1:I:2171:A:HO2'	1:I:2172:U:H5'	1.86	0.40
1:I:2184:A:H2'	1:I:2185:U:C6	2.56	0.40
21:f:15:GLY:HA3	21:f:29:PHE:HE1	1.87	0.40
29:n:14:A:N1	29:n:22:A:O2'	2.55	0.40
30:C:408:A:H1'	30:C:409:U:P	2.62	0.40
30:C:628:G:H2'	30:C:629:A:C8	2.56	0.40
30:C:1039:G:H4'	30:C:1039:G:OP1	2.21	0.40
30:C:1228:C:N4	42:r:103:LYS:O	2.46	0.40
31:D:196:VAL:HB	31:D:199:VAL:HG22	2.02	0.40
37:P:103:VAL:HG12	37:P:126:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:s:53:ARG:O	43:s:59:ARG:HD3	2.21	0.40
1:I:330:A:H2'	1:I:330:A:N3	2.37	0.40
1:I:488:G:H4'	16:a:49:LYS:HE3	2.04	0.40
1:I:1802:A:H8	1:I:1802:A:O5'	2.05	0.40
1:I:1878:G:H2'	1:I:1879:C:O4'	2.22	0.40
1:I:2322:A:H2'	1:I:2323:G:O4'	2.21	0.40
1:I:2649:C:H2'	1:I:2650:U:C6	2.56	0.40
2:J:65:U:H3'	2:J:108:A:N6	2.35	0.40
3:K:77:VAL:HG12	3:K:115:GLN:HG2	2.03	0.40
17:b:14:PRO:HD3	22:g:30:MET:SD	2.62	0.40
27:l:55:LEU:O	27:l:59:ILE:HG13	2.21	0.40
29:n:19:G:O6	29:n:56:U:H1'	2.21	0.40
30:C:161:A:H2'	30:C:162:A:C8	2.56	0.40
30:C:496:A:H2'	30:C:496:A:N3	2.37	0.40
30:C:519:C:OP2	41:q:47:SER:OG	2.37	0.40
30:C:790:A:H2'	30:C:791:G:C8	2.57	0.40
30:C:1045:C:H2'	30:C:1046:A:O4'	2.22	0.40
30:C:1220:G:O3'	48:x:36:ARG:HD3	2.22	0.40
30:C:1272:G:H2'	30:C:1273:C:O4'	2.21	0.40
42:r:5:ALA:HB2	42:r:60:VAL:HG11	2.03	0.40
46:v:30:LYS:HA	46:v:37:PHE:HA	2.01	0.40
46:v:46:VAL:HG21	46:v:61:ILE:HG21	2.04	0.40
1:I:3:U:H2'	1:I:4:U:C6	2.56	0.40
1:I:379:G:O4'	1:I:2232:C:H5''	2.22	0.40
1:I:422:A:H2'	1:I:423:A:O4'	2.21	0.40
1:I:424:G:H2'	1:I:425:G:O4'	2.20	0.40
1:I:544:C:C2'	1:I:545:U:H5'	2.52	0.40
1:I:674:G:H5''	5:M:71:GLY:H	1.86	0.40
1:I:1149:G:H2'	1:I:1150:C:C6	2.56	0.40
1:I:1838:C:H4'	1:I:1839:G:C8	2.57	0.40
1:I:1901:A:OP2	1:I:1901:A:H4'	2.22	0.40
1:I:2040:G:H2'	1:I:2041:U:O4'	2.20	0.40
1:I:2723:C:H2'	1:I:2724:U:O4'	2.20	0.40
7:R:26:GLY:O	7:R:30:THR:HG23	2.21	0.40
7:R:73:VAL:CG1	7:R:86:GLN:HB2	2.52	0.40
9:T:62:PRO:HB2	27:l:25:LYS:HD3	2.04	0.40
14:Y:74:ILE:HD12	14:Y:114:LYS:HG2	2.02	0.40
18:c:86:ARG:NH2	18:c:100:SER:O	2.55	0.40
28:m:2:LYS:HB2	28:m:35:GLN:HG2	2.03	0.40
29:n:25:U:H2'	29:n:26:C:O4'	2.21	0.40
30:C:575:G:O2'	30:C:821:G:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:779:C:H2'	30:C:780:A:O4'	2.22	0.40
30:C:1169:A:H2'	30:C:1170:A:C8	2.56	0.40
30:C:1217:C:OP2	43:s:9:ARG:NH2	2.53	0.40
31:D:187:VAL:HG13	31:D:191:SER:HB3	2.03	0.40
33:F:23:SER:OG	33:F:110:THR:HA	2.22	0.40
33:F:190:ASP:OD1	33:F:190:ASP:N	2.54	0.40
34:G:156:LYS:HG3	34:G:157:ARG:N	2.36	0.40
37:P:89:LYS:HB2	37:P:89:LYS:NZ	2.36	0.40
46:v:5:ILE:HG12	46:v:7:THR:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	269/273 (98%)	255 (95%)	13 (5%)	1 (0%)	30	65
4	L	207/209 (99%)	194 (94%)	12 (6%)	1 (0%)	24	60
5	M	183/201 (91%)	173 (94%)	9 (5%)	1 (0%)	24	60
6	O	64/177 (36%)	60 (94%)	4 (6%)	0	100	100
8	S	38/123 (31%)	37 (97%)	1 (3%)	0	100	100
10	U	10/136 (7%)	10 (100%)	0	0	100	100
11	V	67/127 (53%)	61 (91%)	6 (9%)	0	100	100
12	W	65/117 (56%)	61 (94%)	4 (6%)	0	100	100
13	X	23/115 (20%)	22 (96%)	1 (4%)	0	100	100
16	a	25/110 (23%)	17 (68%)	5 (20%)	3 (12%)	0	1
20	e	68/85 (80%)	65 (96%)	3 (4%)	0	100	100
21	f	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
22	g	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	h	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	6	31
24	i	54/57 (95%)	51 (94%)	1 (2%)	2 (4%)	2	15
25	j	48/55 (87%)	44 (92%)	4 (8%)	0	100	100
26	k	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
27	l	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
28	m	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
31	D	94/241 (39%)	91 (97%)	3 (3%)	0	100	100
32	E	163/233 (70%)	155 (95%)	7 (4%)	1 (1%)	21	56
33	F	203/206 (98%)	172 (85%)	20 (10%)	11 (5%)	1	9
34	G	154/167 (92%)	142 (92%)	11 (7%)	1 (1%)	21	56
35	H	101/135 (75%)	94 (93%)	6 (6%)	1 (1%)	12	45
36	N	151/179 (84%)	144 (95%)	7 (5%)	0	100	100
37	P	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
38	Q	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
39	o	96/103 (93%)	90 (94%)	4 (4%)	2 (2%)	5	27
40	p	115/129 (89%)	104 (90%)	10 (9%)	1 (1%)	14	48
41	q	121/124 (98%)	112 (93%)	7 (6%)	2 (2%)	7	32
42	r	113/118 (96%)	107 (95%)	5 (4%)	1 (1%)	14	48
43	s	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	12	45
44	t	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
45	u	79/82 (96%)	71 (90%)	7 (9%)	1 (1%)	9	38
46	v	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
47	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
48	x	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
49	y	84/87 (97%)	84 (100%)	0	0	100	100
50	5	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
52	z	2/16 (12%)	0	2 (100%)	0	100	100
All	All	3657/4726 (77%)	3424 (94%)	201 (6%)	32 (1%)	16	48

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	a	64	ALA

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Mol	Chain	Res	Type
33	F	151	LYS
33	F	154	ARG
35	H	33	GLU
33	F	28	ILE
33	F	33	LYS
33	F	108	GLY
33	F	152	GLN
33	F	155	VAL
33	F	158	ALA
39	o	57	VAL
16	a	65	ASP
24	i	26	THR
33	F	109	ALA
3	K	157	SER
4	L	19	GLY
32	E	206	GLU
40	p	16	VAL
45	u	80	LYS
16	a	63	GLY
22	g	46	VAL
24	i	55	ILE
33	F	85	ASN
33	F	149	ALA
41	q	44	LYS
41	q	45	PRO
42	r	99	GLY
5	M	83	VAL
23	h	4	THR
43	s	31	ILE
39	o	39	PRO
34	G	108	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	216/218 (99%)	214 (99%)	2 (1%)	70	85
4	L	164/164 (100%)	158 (96%)	6 (4%)	30	64
5	M	165/165 (100%)	161 (98%)	4 (2%)	43	73
6	O	137/138 (99%)	131 (96%)	6 (4%)	25	60
7	R	116/116 (100%)	113 (97%)	3 (3%)	40	72
8	S	103/104 (99%)	100 (97%)	3 (3%)	37	70
9	T	103/103 (100%)	99 (96%)	4 (4%)	28	62
10	U	109/109 (100%)	108 (99%)	1 (1%)	70	85
11	V	100/103 (97%)	98 (98%)	2 (2%)	48	76
12	W	86/87 (99%)	76 (88%)	10 (12%)	5	23
13	X	99/100 (99%)	94 (95%)	5 (5%)	21	55
14	Y	89/90 (99%)	87 (98%)	2 (2%)	45	74
15	Z	84/84 (100%)	82 (98%)	2 (2%)	43	73
16	a	93/93 (100%)	91 (98%)	2 (2%)	45	74
17	b	80/84 (95%)	77 (96%)	3 (4%)	29	63
18	c	83/85 (98%)	77 (93%)	6 (7%)	13	43
19	d	78/78 (100%)	75 (96%)	3 (4%)	29	63
20	e	56/63 (89%)	54 (96%)	2 (4%)	31	65
21	f	67/68 (98%)	66 (98%)	1 (2%)	57	80
22	g	54/55 (98%)	51 (94%)	3 (6%)	19	52
23	h	48/49 (98%)	47 (98%)	1 (2%)	47	75
24	i	47/48 (98%)	45 (96%)	2 (4%)	26	60
25	j	45/49 (92%)	42 (93%)	3 (7%)	15	46
26	k	38/38 (100%)	35 (92%)	3 (8%)	11	39
27	l	51/52 (98%)	49 (96%)	2 (4%)	28	62
28	m	34/34 (100%)	34 (100%)	0	100	100
31	D	186/199 (94%)	179 (96%)	7 (4%)	29	63
32	E	170/190 (90%)	162 (95%)	8 (5%)	23	58
33	F	172/173 (99%)	149 (87%)	23 (13%)	4	18
34	G	119/126 (94%)	116 (98%)	3 (2%)	42	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	H	90/116 (78%)	89 (99%)	1 (1%)	65	83
36	N	126/147 (86%)	121 (96%)	5 (4%)	28	62
37	P	104/105 (99%)	101 (97%)	3 (3%)	37	70
38	Q	105/107 (98%)	102 (97%)	3 (3%)	37	70
39	o	86/90 (96%)	82 (95%)	4 (5%)	23	58
40	p	90/99 (91%)	85 (94%)	5 (6%)	19	52
41	q	103/104 (99%)	101 (98%)	2 (2%)	50	76
42	r	93/96 (97%)	89 (96%)	4 (4%)	26	60
43	s	83/84 (99%)	82 (99%)	1 (1%)	63	82
44	t	76/77 (99%)	74 (97%)	2 (3%)	40	72
45	u	65/65 (100%)	64 (98%)	1 (2%)	57	80
46	v	73/78 (94%)	70 (96%)	3 (4%)	27	61
47	w	57/65 (88%)	56 (98%)	1 (2%)	51	77
48	x	72/79 (91%)	69 (96%)	3 (4%)	26	61
49	y	65/66 (98%)	64 (98%)	1 (2%)	57	80
50	5	60/61 (98%)	56 (93%)	4 (7%)	15	46
52	z	1/1 (100%)	1 (100%)	0	100	100
All	All	4341/4505 (96%)	4176 (96%)	165 (4%)	30	63

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	74	ILE
3	K	271	ARG
4	L	1	MET
4	L	74	GLU
4	L	81	GLU
4	L	105	LYS
4	L	177	VAL
4	L	180	VAL
5	M	5	LEU
5	M	6	LYS
5	M	130	LYS
5	M	165	HIS
6	O	25	THR
6	O	72	LEU

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Mol	Chain	Res	Type
6	O	107	LEU
6	O	114	ASP
6	O	155	GLU
6	O	168	VAL
7	R	1	MET
7	R	17	VAL
7	R	69	ARG
8	S	32	TYR
8	S	35	VAL
8	S	113	MET
9	T	89	VAL
9	T	103	ILE
9	T	116	VAL
9	T	125	LEU
10	U	6	ARG
11	V	13	ASN
11	V	100	CYS
12	W	4	LYS
12	W	16	ARG
12	W	17	LYS
12	W	31	THR
12	W	47	VAL
12	W	54	VAL
12	W	63	LYS
12	W	76	LYS
12	W	85	LYS
12	W	106	LEU
13	X	6	LYS
13	X	27	GLU
13	X	32	VAL
13	X	106	LYS
13	X	111	LYS
14	Y	71	GLN
14	Y	112	LYS
15	Z	37	GLU
15	Z	46	GLU
16	a	68	ASP
16	a	70	LYS
17	b	31	VAL
17	b	72	GLN
17	b	93	LEU
18	c	18	ASP

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Mol	Chain	Res	Type
18	c	26	LYS
18	c	33	LYS
18	c	34	VAL
18	c	46	GLN
18	c	74	ASN
19	d	1	MET
19	d	8	VAL
19	d	77	VAL
20	e	41	ARG
20	e	68	LYS
21	f	56	MET
22	g	2	LYS
22	g	4	LYS
22	g	28	LEU
23	h	16	ARG
24	i	25	VAL
24	i	53	LYS
25	j	17	THR
25	j	32	GLU
25	j	38	LYS
26	k	29	GLN
26	k	39	ARG
26	k	46	LYS
27	l	16	LYS
27	l	25	LYS
31	D	23	TRP
31	D	93	ASN
31	D	100	MET
31	D	129	LEU
31	D	143	LYS
31	D	167	ASP
31	D	174	LYS
32	E	28	GLU
32	E	58	GLU
32	E	84	VAL
32	E	86	LYS
32	E	111	LEU
32	E	127	ARG
32	E	178	LEU
32	E	185	ASN
33	F	17	THR
33	F	28	ILE

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Mol	Chain	Res	Type
33	F	30	THR
33	F	31	LYS
33	F	33	LYS
33	F	60	LYS
33	F	104	ARG
33	F	105	MET
33	F	110	THR
33	F	113	GLU
33	F	124	MET
33	F	125	VAL
33	F	128	ARG
33	F	143	VAL
33	F	154	ARG
33	F	155	VAL
33	F	159	LEU
33	F	169	THR
33	F	183	LYS
33	F	188	ARG
33	F	190	ASP
33	F	192	SER
33	F	196	ASN
34	G	38	VAL
34	G	116	GLU
34	G	164	ILE
35	H	55	HIS
36	N	57	SER
36	N	75	VAL
36	N	97	ASN
36	N	135	VAL
36	N	144	MET
37	P	56	LYS
37	P	89	LYS
37	P	117	ARG
38	Q	27	LYS
38	Q	85	ARG
38	Q	100	LYS
39	o	5	ARG
39	o	27	GLU
39	o	30	LYS
39	o	91	ASP
40	p	16	VAL
40	p	17	SER

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Mol	Chain	Res	Type
40	p	81	ASN
40	p	85	MET
40	p	94	GLU
41	q	52	VAL
41	q	111	LYS
42	r	16	VAL
42	r	42	ASP
42	r	44	LYS
42	r	83	LEU
43	s	39	GLU
44	t	3	LEU
44	t	64	ARG
45	u	45	GLU
46	v	7	THR
46	v	13	VAL
46	v	18	GLU
47	w	35	GLU
48	x	6	LYS
48	x	31	LEU
48	x	64	ASP
49	y	85	LYS
50	5	3	VAL
50	5	44	GLU
50	5	60	LEU
50	5	63	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	200	HIS
5	M	9	GLN
5	M	115	GLN
7	R	58	ASN
7	R	80	HIS
10	U	13	HIS
12	W	29	HIS
14	Y	71	GLN
17	b	48	GLN
21	f	36	HIS
31	D	42	ASN
31	D	58	ASN
31	D	120	GLN

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Mol	Chain	Res	Type
31	D	168	HIS
32	E	123	GLN
33	F	40	GLN
33	F	54	GLN
34	G	12	GLN
34	G	73	ASN
34	G	132	ASN
34	G	148	ASN
35	H	58	HIS
35	H	68	GLN
39	o	15	HIS
40	p	81	ASN
45	u	26	ASN
45	u	40	ASN
45	u	59	HIS
45	u	79	ASN
47	w	54	GLN
49	y	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2896/2904 (99%)	549 (18%)	60 (2%)
2	J	117/118 (99%)	31 (26%)	7 (5%)
29	n	75/76 (98%)	27 (36%)	0
30	C	1516/1533 (98%)	306 (20%)	39 (2%)
51	6	2/3 (66%)	0	0
All	All	4606/4634 (99%)	913 (19%)	106 (2%)

All (913) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	10	A
1	I	23	G
1	I	27	G
1	I	34	U
1	I	42	A
1	I	46	G
1	I	50	U
1	I	55	G
1	I	61	C

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Mol	Chain	Res	Type
1	I	63	A
1	I	71	A
1	I	74	A
1	I	75	G
1	I	79	C
1	I	83	A
1	I	84	A
1	I	86	G
1	I	96	C
1	I	102	U
1	I	118	A
1	I	119	A
1	I	120	U
1	I	131	A
1	I	137	U
1	I	138	U
1	I	139	U
1	I	140	C
1	I	141	G
1	I	142	A
1	I	163	C
1	I	165	A
1	I	177	G
1	I	178	G
1	I	181	A
1	I	196	A
1	I	199	A
1	I	200	U
1	I	216	A
1	I	222	A
1	I	224	U
1	I	233	A
1	I	248	G
1	I	250	G
1	I	265	A
1	I	266	G
1	I	272	A
1	I	275	C
1	I	276	U
1	I	277	G
1	I	278	A
1	I	279	A

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Mol	Chain	Res	Type
1	I	288	U
1	I	311	A
1	I	317	G
1	I	324	A
1	I	329	G
1	I	330	A
1	I	345	A
1	I	354	A
1	I	355	U
1	I	360	U
1	I	361	G
1	I	362	A
1	I	367	G
1	I	369	U
1	I	370	G
1	I	371	A
1	I	372	G
1	I	386	G
1	I	390	U
1	I	396	G
1	I	397	U
1	I	404	A
1	I	405	U
1	I	411	G
1	I	412	A
1	I	424	G
1	I	434	U
1	I	435	C
1	I	445	C
1	I	451	U
1	I	454	A
1	I	467	G
1	I	474	G
1	I	475	C
1	I	480	A
1	I	481	G
1	I	491	G
1	I	496	G
1	I	504	A
1	I	505	A
1	I	509	C
1	I	512	G

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Mol	Chain	Res	Type
1	I	513	A
1	I	528	A
1	I	532	A
1	I	545	U
1	I	546	U
1	I	547	A
1	I	548	G
1	I	549	G
1	I	554	U
1	I	563	A
1	I	573	U
1	I	575	A
1	I	603	A
1	I	613	A
1	I	614	A
1	I	615	U
1	I	620	G
1	I	621	A
1	I	627	A
1	I	637	A
1	I	638	G
1	I	645	C
1	I	647	G
1	I	651	G
1	I	654	A
1	I	655	A
1	I	668	A
1	I	686	U
1	I	703	U
1	I	717	C
1	I	727	A
1	I	730	A
1	I	746	PSU
1	I	747	5MU
1	I	764	A
1	I	775	G
1	I	776	G
1	I	782	A
1	I	784	G
1	I	785	G
1	I	791	C
1	I	793	A

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Mol	Chain	Res	Type
1	I	804	A
1	I	805	G
1	I	812	C
1	I	819	A
1	I	827	U
1	I	828	U
1	I	831	G
1	I	845	A
1	I	846	U
1	I	847	U
1	I	858	G
1	I	869	G
1	I	877	A
1	I	878	A
1	I	880	G
1	I	896	A
1	I	897	C
1	I	905	A
1	I	907	G
1	I	910	A
1	I	931	U
1	I	932	U
1	I	941	A
1	I	946	C
1	I	958	U
1	I	961	C
1	I	974	G
1	I	983	A
1	I	984	A
1	I	985	C
1	I	995	C
1	I	996	A
1	I	1003	G
1	I	1012	U
1	I	1013	C
1	I	1026	G
1	I	1033	U
1	I	1043	C
1	I	1046	A
1	I	1047	G
1	I	1051	G
1	I	1060	U

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Mol	Chain	Res	Type
1	I	1061	U
1	I	1069	A
1	I	1070	A
1	I	1071	G
1	I	1073	A
1	I	1079	C
1	I	1083	U
1	I	1084	A
1	I	1086	A
1	I	1088	A
1	I	1097	U
1	I	1098	A
1	I	1102	C
1	I	1107	G
1	I	1110	G
1	I	1111	A
1	I	1112	G
1	I	1116	G
1	I	1119	U
1	I	1128	G
1	I	1129	A
1	I	1131	G
1	I	1132	U
1	I	1133	A
1	I	1134	A
1	I	1135	C
1	I	1136	G
1	I	1142	A
1	I	1157	G
1	I	1170	C
1	I	1173	U
1	I	1174	U
1	I	1175	A
1	I	1176	U
1	I	1180	U
1	I	1182	G
1	I	1226	A
1	I	1236	G
1	I	1237	A
1	I	1238	G
1	I	1247	A
1	I	1248	G

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Mol	Chain	Res	Type
1	I	1250	G
1	I	1253	A
1	I	1256	G
1	I	1266	G
1	I	1271	G
1	I	1272	A
1	I	1275	A
1	I	1288	G
1	I	1289	C
1	I	1294	U
1	I	1300	G
1	I	1301	A
1	I	1302	A
1	I	1303	G
1	I	1306	C
1	I	1312	U
1	I	1315	C
1	I	1320	C
1	I	1321	A
1	I	1329	U
1	I	1340	U
1	I	1341	G
1	I	1342	A
1	I	1344	U
1	I	1345	C
1	I	1352	U
1	I	1359	A
1	I	1360	G
1	I	1365	A
1	I	1368	G
1	I	1379	U
1	I	1383	A
1	I	1386	C
1	I	1395	A
1	I	1407	G
1	I	1416	G
1	I	1417	C
1	I	1420	A
1	I	1421	G
1	I	1427	A
1	I	1428	C
1	I	1437	C

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Mol	Chain	Res	Type
1	I	1451	C
1	I	1453	A
1	I	1458	U
1	I	1459	G
1	I	1461	C
1	I	1475	G
1	I	1482	G
1	I	1489	C
1	I	1490	A
1	I	1491	G
1	I	1493	C
1	I	1494	A
1	I	1508	A
1	I	1509	A
1	I	1510	G
1	I	1515	A
1	I	1523	U
1	I	1532	A
1	I	1533	C
1	I	1534	U
1	I	1535	A
1	I	1536	C
1	I	1537	G
1	I	1540	G
1	I	1554	U
1	I	1569	A
1	I	1578	U
1	I	1582	C
1	I	1583	A
1	I	1584	U
1	I	1585	C
1	I	1588	G
1	I	1602	U
1	I	1607	C
1	I	1608	A
1	I	1610	A
1	I	1613	G
1	I	1618	A
1	I	1619	G
1	I	1622	G
1	I	1626	A
1	I	1634	A

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Mol	Chain	Res	Type
1	I	1647	U
1	I	1648	U
1	I	1649	G
1	I	1653	G
1	I	1667	G
1	I	1669	A
1	I	1674	G
1	I	1681	G
1	I	1694	C
1	I	1700	A
1	I	1715	G
1	I	1721	G
1	I	1724	G
1	I	1729	U
1	I	1730	C
1	I	1731	G
1	I	1732	C
1	I	1738	G
1	I	1758	U
1	I	1764	C
1	I	1773	A
1	I	1784	A
1	I	1788	C
1	I	1800	C
1	I	1801	A
1	I	1802	A
1	I	1807	G
1	I	1808	A
1	I	1809	A
1	I	1816	C
1	I	1818	U
1	I	1829	A
1	I	1833	C
1	I	1847	A
1	I	1857	G
1	I	1864	U
1	I	1869	G
1	I	1870	C
1	I	1871	A
1	I	1872	A
1	I	1873	G
1	I	1884	G

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Mol	Chain	Res	Type
1	I	1906	G
1	I	1914	C
1	I	1929	G
1	I	1936	A
1	I	1938	A
1	I	1940	U
1	I	1955	U
1	I	1967	C
1	I	1970	A
1	I	1971	U
1	I	1972	G
1	I	1991	U
1	I	1992	G
1	I	1993	U
1	I	1997	C
1	I	2020	A
1	I	2022	U
1	I	2023	C
1	I	2025	C
1	I	2031	A
1	I	2036	C
1	I	2043	C
1	I	2049	G
1	I	2051	A
1	I	2055	C
1	I	2056	G
1	I	2060	A
1	I	2061	G
1	I	2062	A
1	I	2063	C
1	I	2069	G
1	I	2072	C
1	I	2078	C
1	I	2102	G
1	I	2110	G
1	I	2111	U
1	I	2112	G
1	I	2113	U
1	I	2114	A
1	I	2115	G
1	I	2116	G
1	I	2117	A

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Mol	Chain	Res	Type
1	I	2118	U
1	I	2119	A
1	I	2120	G
1	I	2124	G
1	I	2125	G
1	I	2126	A
1	I	2127	G
1	I	2128	G
1	I	2132	U
1	I	2133	G
1	I	2134	A
1	I	2141	G
1	I	2142	A
1	I	2147	A
1	I	2157	G
1	I	2158	A
1	I	2162	G
1	I	2163	A
1	I	2164	C
1	I	2170	A
1	I	2171	A
1	I	2172	U
1	I	2173	A
1	I	2181	U
1	I	2183	A
1	I	2189	U
1	I	2198	A
1	I	2204	G
1	I	2210	U
1	I	2211	A
1	I	2212	A
1	I	2224	G
1	I	2225	A
1	I	2238	G
1	I	2239	G
1	I	2249	U
1	I	2268	A
1	I	2279	G
1	I	2282	G
1	I	2283	C
1	I	2288	A
1	I	2289	G

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Mol	Chain	Res	Type
1	I	2296	U
1	I	2297	A
1	I	2305	U
1	I	2307	G
1	I	2308	G
1	I	2309	A
1	I	2317	A
1	I	2319	G
1	I	2320	U
1	I	2322	A
1	I	2324	U
1	I	2325	G
1	I	2327	A
1	I	2331	G
1	I	2333	A
1	I	2335	A
1	I	2336	A
1	I	2347	C
1	I	2350	C
1	I	2375	G
1	I	2383	G
1	I	2384	U
1	I	2385	C
1	I	2389	G
1	I	2396	G
1	I	2402	U
1	I	2406	A
1	I	2410	G
1	I	2423	U
1	I	2424	C
1	I	2425	A
1	I	2426	A
1	I	2428	G
1	I	2429	G
1	I	2430	A
1	I	2431	U
1	I	2434	A
1	I	2435	A
1	I	2441	U
1	I	2448	A
1	I	2470	G
1	I	2476	A

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Mol	Chain	Res	Type
1	I	2478	A
1	I	2481	G
1	I	2484	G
1	I	2491	U
1	I	2494	G
1	I	2498	OMC
1	I	2502	G
1	I	2505	G
1	I	2513	A
1	I	2517	C
1	I	2518	A
1	I	2529	G
1	I	2535	G
1	I	2547	A
1	I	2549	G
1	I	2554	U
1	I	2566	A
1	I	2567	G
1	I	2573	C
1	I	2581	G
1	I	2582	G
1	I	2583	G
1	I	2585	U
1	I	2602	A
1	I	2603	G
1	I	2609	U
1	I	2613	U
1	I	2629	U
1	I	2630	G
1	I	2645	G
1	I	2646	C
1	I	2656	U
1	I	2663	G
1	I	2681	C
1	I	2682	A
1	I	2685	G
1	I	2689	U
1	I	2690	U
1	I	2714	G
1	I	2716	C
1	I	2718	G
1	I	2726	A

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Mol	Chain	Res	Type
1	I	2732	G
1	I	2733	A
1	I	2739	U
1	I	2744	G
1	I	2748	A
1	I	2750	A
1	I	2752	C
1	I	2757	A
1	I	2758	A
1	I	2765	A
1	I	2777	G
1	I	2778	A
1	I	2781	A
1	I	2791	G
1	I	2792	A
1	I	2793	C
1	I	2794	C
1	I	2798	U
1	I	2799	A
1	I	2800	A
1	I	2809	A
1	I	2820	A
1	I	2823	A
1	I	2835	A
1	I	2836	U
1	I	2867	G
1	I	2873	A
1	I	2874	C
1	I	2880	C
1	I	2883	A
1	I	2884	U
1	I	2893	A
1	I	2895	G
1	I	2898	U
1	I	2903	U
1	I	2904	U
2	J	4	C
2	J	9	G
2	J	12	C
2	J	13	G
2	J	14	U
2	J	15	A

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Mol	Chain	Res	Type
2	J	16	G
2	J	20	G
2	J	21	G
2	J	24	G
2	J	25	U
2	J	27	C
2	J	32	U
2	J	34	A
2	J	35	C
2	J	36	C
2	J	37	C
2	J	41	G
2	J	42	C
2	J	45	A
2	J	52	A
2	J	53	A
2	J	56	G
2	J	57	A
2	J	66	A
2	J	67	G
2	J	88	C
2	J	89	U
2	J	90	C
2	J	108	A
2	J	109	A
29	n	3	C
29	n	5	G
29	n	9	G
29	n	10	G
29	n	11	A
29	n	14	A
29	n	15	G
29	n	16	C
29	n	17	C
29	n	18	U
29	n	19	G
29	n	20	G
29	n	21	U
29	n	22	A
29	n	23	G
29	n	29	C
29	n	48	U

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Mol	Chain	Res	Type
29	n	49	C
29	n	54	G
29	n	55	U
29	n	59	A
29	n	60	A
29	n	61	U
29	n	62	C
29	n	68	C
29	n	70	C
29	n	77	A
30	C	3	A
30	C	4	U
30	C	5	U
30	C	7	A
30	C	8	A
30	C	9	G
30	C	22	G
30	C	31	G
30	C	32	A
30	C	39	G
30	C	47	C
30	C	48	C
30	C	51	A
30	C	59	A
30	C	70	U
30	C	71	A
30	C	73	C
30	C	74	A
30	C	75	G
30	C	81	A
30	C	82	G
30	C	83	C
30	C	84	U
30	C	85	U
30	C	86	G
30	C	87	C
30	C	93	U
30	C	94	G
30	C	95	C
30	C	99	C
30	C	116	A
30	C	120	A

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Mol	Chain	Res	Type
30	C	122	G
30	C	131	A
30	C	141	G
30	C	143	A
30	C	149	A
30	C	173	U
30	C	177	G
30	C	182	A
30	C	183	C
30	C	191	G
30	C	197	A
30	C	240	G
30	C	245	U
30	C	247	G
30	C	251	G
30	C	253	A
30	C	266	G
30	C	267	C
30	C	289	G
30	C	315	A
30	C	316	C
30	C	328	C
30	C	329	A
30	C	330	C
30	C	352	C
30	C	354	G
30	C	355	C
30	C	367	U
30	C	372	C
30	C	374	A
30	C	398	U
30	C	406	G
30	C	409	U
30	C	411	A
30	C	412	A
30	C	413	G
30	C	414	A
30	C	415	A
30	C	416	G
30	C	418	C
30	C	419	C
30	C	420	U

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Mol	Chain	Res	Type
30	C	421	U
30	C	422	C
30	C	423	G
30	C	425	G
30	C	426	U
30	C	427	U
30	C	428	G
30	C	429	U
30	C	431	A
30	C	432	A
30	C	434	U
30	C	435	A
30	C	436	C
30	C	437	U
30	C	438	U
30	C	439	U
30	C	446	G
30	C	447	G
30	C	448	A
30	C	452	A
30	C	457	G
30	C	458	U
30	C	459	A
30	C	462	G
30	C	464	U
30	C	465	A
30	C	467	U
30	C	468	A
30	C	478	A
30	C	479	U
30	C	481	G
30	C	482	A
30	C	484	G
30	C	486	U
30	C	495	A
30	C	496	A
30	C	498	A
30	C	499	A
30	C	500	G
30	C	509	A
30	C	511	C
30	C	515	G

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Mol	Chain	Res	Type
30	C	516	U
30	C	518	C
30	C	524	G
30	C	527	G
30	C	531	U
30	C	532	A
30	C	533	A
30	C	536	C
30	C	537	G
30	C	538	G
30	C	539	A
30	C	542	G
30	C	543	U
30	C	544	G
30	C	545	C
30	C	547	A
30	C	559	A
30	C	560	A
30	C	562	U
30	C	564	C
30	C	572	A
30	C	573	A
30	C	576	C
30	C	579	A
30	C	596	A
30	C	597	G
30	C	611	C
30	C	613	C
30	C	614	C
30	C	615	G
30	C	616	G
30	C	617	G
30	C	618	C
30	C	626	G
30	C	628	G
30	C	633	G
30	C	641	U
30	C	642	A
30	C	650	G
30	C	653	U
30	C	665	A
30	C	687	A

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Mol	Chain	Res	Type
30	C	695	A
30	C	702	A
30	C	703	G
30	C	720	C
30	C	721	G
30	C	722	G
30	C	723	U
30	C	724	G
30	C	747	A
30	C	748	G
30	C	755	G
30	C	759	A
30	C	777	A
30	C	793	U
30	C	794	A
30	C	809	G
30	C	815	A
30	C	817	C
30	C	819	A
30	C	832	G
30	C	851	G
30	C	867	G
30	C	873	A
30	C	874	G
30	C	884	U
30	C	885	G
30	C	887	G
30	C	890	G
30	C	902	G
30	C	914	A
30	C	926	G
30	C	934	C
30	C	935	A
30	C	960	U
30	C	969	A
30	C	975	A
30	C	976	G
30	C	977	A
30	C	989	U
30	C	992	U
30	C	993	G
30	C	994	A

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Mol	Chain	Res	Type
30	C	996	A
30	C	1003	G
30	C	1004	A
30	C	1008	U
30	C	1009	U
30	C	1010	U
30	C	1022	A
30	C	1030	U
30	C	1031	C
30	C	1032	G
30	C	1033	G
30	C	1034	G
30	C	1035	A
30	C	1036	A
30	C	1039	G
30	C	1042	A
30	C	1046	A
30	C	1063	C
30	C	1064	G
30	C	1065	U
30	C	1066	C
30	C	1085	U
30	C	1089	G
30	C	1094	G
30	C	1095	U
30	C	1101	A
30	C	1129	C
30	C	1130	A
30	C	1132	C
30	C	1134	G
30	C	1135	U
30	C	1137	C
30	C	1139	G
30	C	1140	C
30	C	1145	A
30	C	1146	A
30	C	1157	A
30	C	1160	G
30	C	1167	A
30	C	1176	A
30	C	1184	G
30	C	1196	A

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Mol	Chain	Res	Type
30	C	1197	A
30	C	1201	A
30	C	1206	G
30	C	1207	G
30	C	1211	U
30	C	1212	U
30	C	1213	A
30	C	1214	C
30	C	1227	A
30	C	1238	A
30	C	1248	A
30	C	1256	A
30	C	1257	A
30	C	1260	G
30	C	1261	A
30	C	1270	G
30	C	1275	A
30	C	1280	A
30	C	1286	U
30	C	1287	A
30	C	1289	A
30	C	1290	G
30	C	1291	U
30	C	1297	G
30	C	1298	U
30	C	1300	G
30	C	1302	C
30	C	1305	G
30	C	1317	C
30	C	1332	A
30	C	1336	C
30	C	1337	G
30	C	1338	G
30	C	1340	A
30	C	1346	A
30	C	1353	G
30	C	1363	A
30	C	1368	A
30	C	1370	G
30	C	1378	C
30	C	1379	G
30	C	1381	U

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Mol	Chain	Res	Type
30	C	1396	A
30	C	1397	C
30	C	1398	A
30	C	1419	G
30	C	1432	G
30	C	1439	G
30	C	1441	A
30	C	1451	U
30	C	1452	C
30	C	1453	G
30	C	1454	G
30	C	1492	A
30	C	1493	A
30	C	1494	G
30	C	1497	G
30	C	1499	A
30	C	1503	A
30	C	1506	U
30	C	1516	G
30	C	1517	G
30	C	1529	G
30	C	1530	G

All (106) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	33	C
1	I	62	U
1	I	83	A
1	I	177	G
1	I	196	A
1	I	199	A
1	I	360	U
1	I	361	G
1	I	404	A
1	I	434	U
1	I	474	G
1	I	512	G
1	I	620	G
1	I	764	A
1	I	784	G
1	I	827	U

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Mol	Chain	Res	Type
1	I	830	G
1	I	973	A
1	I	984	A
1	I	989	G
1	I	1060	U
1	I	1069	A
1	I	1110	G
1	I	1128	G
1	I	1131	G
1	I	1288	G
1	I	1320	C
1	I	1324	G
1	I	1344	U
1	I	1395	A
1	I	1536	C
1	I	1554	U
1	I	1608	A
1	I	1647	U
1	I	1730	C
1	I	1870	C
1	I	1980	G
1	I	2110	G
1	I	2112	G
1	I	2116	G
1	I	2126	A
1	I	2133	G
1	I	2146	C
1	I	2282	G
1	I	2288	A
1	I	2308	G
1	I	2318	G
1	I	2324	U
1	I	2425	A
1	I	2430	A
1	I	2517	C
1	I	2581	G
1	I	2602	A
1	I	2609	U
1	I	2645	G
1	I	2681	C
1	I	2756	U
1	I	2797	U

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Mol	Chain	Res	Type
1	I	2873	A
1	I	2903	U
2	J	24	G
2	J	36	C
2	J	41	G
2	J	52	A
2	J	56	G
2	J	88	C
2	J	108	A
30	C	7	A
30	C	70	U
30	C	73	C
30	C	315	A
30	C	408	A
30	C	411	A
30	C	412	A
30	C	418	C
30	C	422	C
30	C	431	A
30	C	434	U
30	C	435	A
30	C	437	U
30	C	438	U
30	C	447	G
30	C	499	A
30	C	535	A
30	C	559	A
30	C	641	U
30	C	686	U
30	C	722	G
30	C	884	U
30	C	993	G
30	C	1003	G
30	C	1034	G
30	C	1035	A
30	C	1039	G
30	C	1094	G
30	C	1124	G
30	C	1129	C
30	C	1134	G
30	C	1145	A
30	C	1211	U

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Mol	Chain	Res	Type
30	C	1225	A
30	C	1278	G
30	C	1297	G
30	C	1298	U
30	C	1337	G
30	C	1447	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
52	MAA	z	4	52	4,5,6	0.47	0	2,5,7	0.84	0
1	2MG	I	1835	1	23,26,27	0.48	0	33,38,41	0.50	0
52	DVA	z	5	52	4,6,7	0.56	0	6,7,9	0.84	0
52	DHV	z	15	52	5,7,8	0.66	0	7,10,12	0.88	0
52	DAL	z	14	52	3,4,5	0.67	0	2,4,6	0.91	0
1	PSU	I	746	1,53	18,21,22	1.11	2 (11%)	21,30,33	1.85	4 (19%)
52	DVA	z	12	52	4,6,7	0.57	0	6,7,9	0.73	0
52	RXL	z	2	52	5,6,7	1.61	2 (40%)	5,7,9	1.14	1 (20%)
1	2MG	I	2445	1	23,26,27	0.54	0	33,38,41	0.57	0
52	DVA	z	6	52	4,6,7	0.58	0	6,7,9	0.80	0
1	PSU	I	1917	1	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
1	OMG	I	2251	1,29	23,26,27	0.53	0	32,38,41	0.53	0
52	RXL	z	9	52	5,6,7	1.66	2 (40%)	5,7,9	1.21	1 (20%)
1	PSU	I	1911	1	18,21,22	1.10	2 (11%)	21,30,33	2.08	6 (28%)
1	OMC	I	2498	1	19,22,23	0.65	0	25,31,34	0.65	0
52	DVA	z	8	52	4,6,7	0.56	0	6,7,9	0.88	0
1	5MU	I	1939	1	19,22,23	0.48	0	27,32,35	0.44	0
1	2MA	I	2503	1	22,25,26	3.98	9 (40%)	32,37,40	2.28	10 (31%)
1	PSU	I	2504	1	18,21,22	1.13	2 (11%)	21,30,33	1.99	6 (28%)
52	IB9	z	7	52	11,12,13	0.25	0	12,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	RX9	z	13	52	6,7,8	1.80	3 (50%)	4,8,10	1.31	1 (25%)
1	5MU	I	747	1	19,22,23	0.57	0	27,32,35	0.49	0
1	PSU	I	2457	1	18,21,22	1.15	2 (11%)	21,30,33	2.19	6 (28%)
52	DAR	z	10	52	9,10,11	0.42	0	5,11,13	0.49	0
1	1MG	I	745	1	23,26,27	3.07	8 (34%)	33,39,42	2.09	11 (33%)
1	PSU	I	955	1	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
1	OMU	I	2552	1	19,22,23	2.96	8 (42%)	25,31,34	1.85	5 (20%)
1	PSU	I	2605	1	18,21,22	1.09	1 (5%)	21,30,33	1.84	3 (14%)
1	5MC	I	1962	1	19,22,23	0.65	0	26,32,35	0.65	0
1	PSU	I	2580	1	18,21,22	1.14	3 (16%)	21,30,33	2.17	7 (33%)

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
52	MAA	z	4	52	-	0/2/4/6	-
1	2MG	I	1835	1	-	0/9/27/28	0/3/3/3
52	DVA	z	5	52	-	0/5/6/8	-
52	DHV	z	15	52	-	0/4/8/10	-
52	DAL	z	14	52	-	0/1/2/4	-
1	PSU	I	746	1,53	-	2/7/25/26	0/2/2/2
52	DVA	z	12	52	-	0/5/6/8	-
52	RXL	z	2	52	-	0/0/6/8	-
1	2MG	I	2445	1	-	0/9/27/28	0/3/3/3
52	DVA	z	6	52	-	1/5/6/8	-
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	I	2251	1,29	-	1/9/27/28	0/3/3/3
52	RXL	z	9	52	-	0/0/6/8	-
1	PSU	I	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	I	2498	1	-	1/9/27/28	0/2/2/2
52	DVA	z	8	52	-	0/5/6/8	-
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	2MA	I	2503	1	-	1/7/25/26	0/3/3/3
1	PSU	I	2504	1	-	2/7/25/26	0/2/2/2
52	IB9	z	7	52	-	0/7/7/8	0/1/1/1
52	RX9	z	13	52	-	0/2/8/10	-
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	DAR	z	10	52	-	3/8/9/11	-
1	1MG	I	745	1	-	0/7/25/26	0/3/3/3
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	I	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2503	2MA	C4-N3	12.45	1.50	1.34
1	I	745	1MG	C2-N3	8.44	1.46	1.33
1	I	2503	2MA	C2-N1	7.13	1.46	1.34
1	I	2552	OMU	C2-N1	6.89	1.49	1.38
1	I	2503	2MA	C2-N3	6.68	1.45	1.34
1	I	2552	OMU	C2-N3	6.54	1.49	1.38
1	I	745	1MG	C4-N3	6.04	1.48	1.34
1	I	745	1MG	C2-N2	5.95	1.44	1.34
1	I	2552	OMU	C6-C5	5.51	1.47	1.35
1	I	2503	2MA	C6-N1	5.49	1.42	1.35
1	I	2503	2MA	C5-C6	4.70	1.54	1.41
1	I	2503	2MA	C5-N7	-4.44	1.31	1.39
1	I	745	1MG	C5-C6	4.19	1.56	1.45
1	I	745	1MG	O6-C6	-4.09	1.14	1.23
1	I	745	1MG	C2-N1	4.08	1.44	1.37
1	I	2552	OMU	C4-N3	3.88	1.45	1.38
1	I	1917	PSU	C6-C5	3.50	1.39	1.35
1	I	2457	PSU	C6-C5	3.40	1.39	1.35
1	I	2504	PSU	C6-C5	3.39	1.39	1.35
1	I	2605	PSU	C6-C5	3.34	1.39	1.35
1	I	955	PSU	C6-C5	3.30	1.38	1.35
1	I	746	PSU	C6-C5	3.29	1.38	1.35
1	I	1911	PSU	C6-C5	3.23	1.38	1.35
1	I	2552	OMU	O4-C4	-3.14	1.18	1.24
1	I	2580	PSU	C6-C5	3.14	1.38	1.35
1	I	2503	2MA	C6-N6	-3.13	1.26	1.34
1	I	745	1MG	C5-N7	-3.07	1.32	1.39
1	I	2552	OMU	C6-N1	2.75	1.44	1.38
52	z	9	RXL	C-CA	-2.68	1.40	1.45
1	I	2552	OMU	O2-C2	-2.65	1.18	1.23
52	z	13	RX9	CB-CA	2.62	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2503	2MA	C4-N9	-2.51	1.32	1.37
1	I	745	1MG	C8-N9	-2.47	1.32	1.37
52	z	2	RXL	C-CA	-2.46	1.40	1.45
52	z	13	RX9	CA-N	2.45	1.42	1.36
52	z	2	RXL	CA-N	2.44	1.42	1.36
1	I	2580	PSU	O4'-C1'	-2.39	1.40	1.43
52	z	9	RXL	CA-N	2.37	1.41	1.36
52	z	13	RX9	C-CA	-2.32	1.41	1.45
1	I	2457	PSU	O4'-C1'	-2.27	1.40	1.43
1	I	2552	OMU	C5-C4	2.22	1.48	1.43
1	I	746	PSU	O4'-C1'	-2.21	1.40	1.43
1	I	2504	PSU	C4-C5	-2.12	1.38	1.44
1	I	1911	PSU	O4'-C1'	-2.09	1.41	1.43
1	I	2580	PSU	C4-C5	-2.06	1.38	1.44
1	I	2503	2MA	C8-N9	-2.00	1.34	1.37

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2503	2MA	C5-C4-N3	-7.34	119.45	127.18
1	I	2552	OMU	C4-N3-C2	-5.86	119.34	126.61
1	I	2457	PSU	N1-C2-N3	5.46	120.93	115.17
1	I	2457	PSU	C4-N3-C2	-5.41	118.91	126.37
1	I	745	1MG	C5-C4-N3	-5.20	120.12	128.39
1	I	2580	PSU	N1-C2-N3	5.13	120.58	115.17
1	I	745	1MG	C1'-N9-C4	-5.04	111.59	126.49
1	I	1911	PSU	C4-N3-C2	-5.03	119.44	126.37
1	I	2580	PSU	C4-N3-C2	-4.96	119.53	126.37
1	I	1911	PSU	N1-C2-N3	4.93	120.37	115.17
1	I	2504	PSU	N1-C2-N3	4.90	120.33	115.17
1	I	955	PSU	C4-N3-C2	-4.89	119.63	126.37
1	I	2605	PSU	C4-N3-C2	-4.87	119.66	126.37
1	I	2504	PSU	C4-N3-C2	-4.84	119.71	126.37
1	I	746	PSU	C4-N3-C2	-4.80	119.76	126.37
1	I	1917	PSU	N1-C2-N3	4.79	120.22	115.17
1	I	1917	PSU	C4-N3-C2	-4.77	119.80	126.37
1	I	955	PSU	N1-C2-N3	4.75	120.18	115.17
1	I	2605	PSU	N1-C2-N3	4.69	120.11	115.17
1	I	745	1MG	C1'-N9-C8	4.68	140.01	126.73
1	I	2503	2MA	N3-C4-N9	4.65	132.89	126.99
1	I	746	PSU	N1-C2-N3	4.51	119.92	115.17
1	I	2503	2MA	N9-C8-N7	-4.11	108.11	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2552	OMU	N3-C2-N1	3.98	120.08	114.89
1	I	2552	OMU	C5-C4-N3	3.83	120.17	114.80
1	I	2503	2MA	N3-C2-N1	-3.61	119.39	125.77
1	I	745	1MG	C2-N3-C4	3.59	120.06	111.98
1	I	745	1MG	N9-C4-N3	3.04	132.03	125.95
1	I	745	1MG	N9-C8-N7	-3.00	107.84	113.40
1	I	2503	2MA	C5-N7-C8	2.96	108.10	103.45
1	I	2580	PSU	O2-C2-N1	-2.93	119.77	122.79
1	I	746	PSU	O2-C2-N1	-2.89	119.81	122.79
1	I	2552	OMU	O4-C4-C5	-2.89	120.19	125.16
1	I	1911	PSU	O2-C2-N1	-2.83	119.87	122.79
1	I	2457	PSU	O2-C2-N1	-2.76	119.94	122.79
1	I	2457	PSU	C6-C5-C4	2.75	120.03	118.17
1	I	2580	PSU	O4'-C1'-C2'	2.74	108.94	105.15
1	I	2503	2MA	C4-N9-C1'	-2.72	120.26	126.63
1	I	1917	PSU	O2-C2-N1	-2.68	120.02	122.79
1	I	745	1MG	C5-C6-N1	2.64	119.90	115.02
1	I	2580	PSU	C6-C5-C4	2.61	119.94	118.17
1	I	2504	PSU	O2-C2-N1	-2.60	120.11	122.79
1	I	2580	PSU	C6-N1-C2	-2.59	120.28	122.69
52	z	13	RX9	O-C-CA	-2.57	120.71	125.53
52	z	2	RXL	O-C-CA	-2.54	120.78	125.53
1	I	2503	2MA	CM2-C2-N1	2.54	120.92	117.13
52	z	9	RXL	O-C-CA	-2.52	120.81	125.53
1	I	955	PSU	O2-C2-N1	-2.48	120.23	122.79
1	I	1911	PSU	O4'-C1'-C2'	2.48	108.58	105.15
1	I	2504	PSU	C6-C5-C4	2.47	119.84	118.17
1	I	2504	PSU	C6-N1-C2	-2.47	120.40	122.69
1	I	1911	PSU	C6-N1-C2	-2.41	120.45	122.69
1	I	1917	PSU	C6-N1-C2	-2.39	120.47	122.69
1	I	1911	PSU	C6-C5-C4	2.39	119.79	118.17
1	I	2457	PSU	O4'-C1'-C2'	2.37	108.43	105.15
1	I	2503	2MA	C6-C5-C4	2.31	120.33	117.18
1	I	2503	2MA	N6-C6-N1	2.28	120.11	117.03
1	I	2457	PSU	C6-N1-C2	-2.23	120.62	122.69
1	I	2580	PSU	C3'-C2'-C1'	2.23	104.32	101.69
1	I	955	PSU	C6-N1-C2	-2.21	120.64	122.69
1	I	2504	PSU	O4'-C1'-C2'	2.19	108.18	105.15
1	I	2503	2MA	C1'-N9-C8	2.18	131.93	127.09
1	I	2605	PSU	C6-N1-C2	-2.18	120.67	122.69
1	I	745	1MG	C8-N7-C5	2.14	108.06	104.26
1	I	745	1MG	CM1-N1-C6	2.13	120.95	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	745	1MG	N2-C2-N1	2.11	120.48	118.79
1	I	1917	PSU	O4'-C1'-C2'	2.04	107.98	105.15
1	I	745	1MG	O6-C6-C5	-2.04	119.33	124.59
1	I	746	PSU	C6-N1-C2	-2.04	120.80	122.69
1	I	2552	OMU	O2-C2-N1	-2.03	120.15	122.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	746	PSU	C2'-C1'-C5-C4
1	I	2251	OMG	C1'-C2'-O2'-CM2
52	z	6	DVA	C-CA-CB-CG2
52	z	10	DAR	NH1-CZ-NE-CD
52	z	10	DAR	NH2-CZ-NE-CD
1	I	2504	PSU	O4'-C4'-C5'-O5'
1	I	2504	PSU	C3'-C4'-C5'-O5'
52	z	10	DAR	CG-CD-NE-CZ
1	I	2498	OMC	O4'-C4'-C5'-O5'
1	I	746	PSU	O4'-C1'-C5-C4
1	I	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	z	5	DVA	3	0
52	z	12	DVA	1	0
1	I	2445	2MG	1	0
52	z	6	DVA	2	0
1	I	2251	OMG	1	0
52	z	9	RXL	1	0
1	I	2498	OMC	2	0
52	z	8	DVA	1	0
1	I	747	5MU	2	0
52	z	10	DAR	1	0
1	I	2552	OMU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 241 ligands modelled in this entry, 238 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	FME	n	101	29	8,9,10	0.76	0	8,9,11	1.15	1 (12%)
56	SPD	C	1689	-	9,9,9	0.35	0	8,8,8	0.66	0
56	SPD	C	1688	-	9,9,9	0.31	0	8,8,8	0.82	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	FME	n	101	29	-	1/7/9/11	-
56	SPD	C	1689	-	-	1/7/7/7	-
56	SPD	C	1688	-	-	0/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	n	101	FME	C-CA-N	2.35	114.04	109.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	C	1689	SPD	C4-C5-N6-C7
55	n	101	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	n	101	FME	6	0
56	C	1689	SPD	3	0
56	C	1688	SPD	2	0

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.

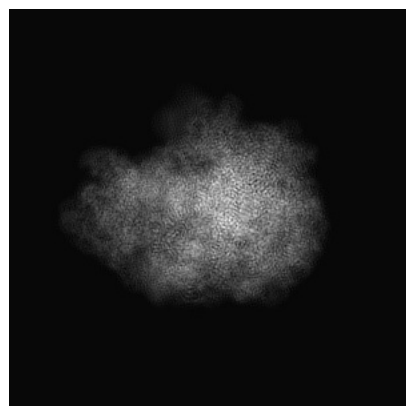
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15905. These allow visual inspection of the internal detail of the map and identification of artifacts.

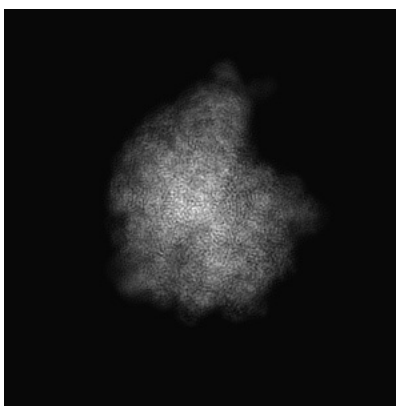
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

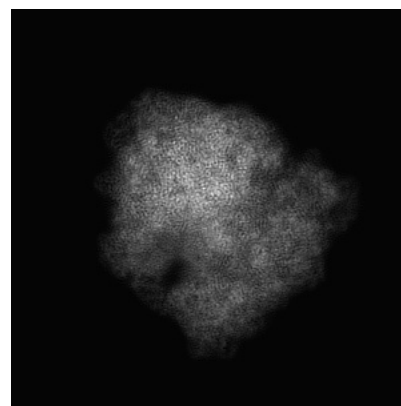
6.1.1 Primary map



X

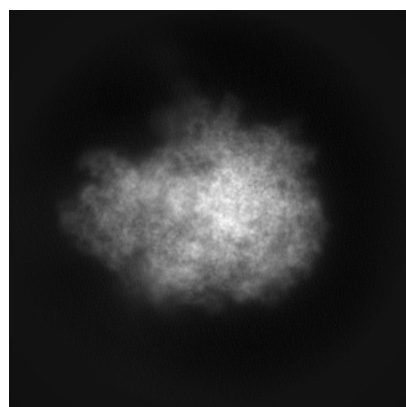


Y

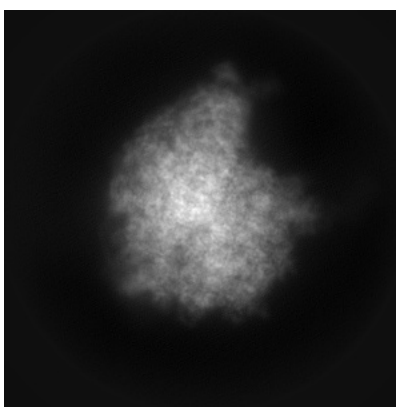


Z

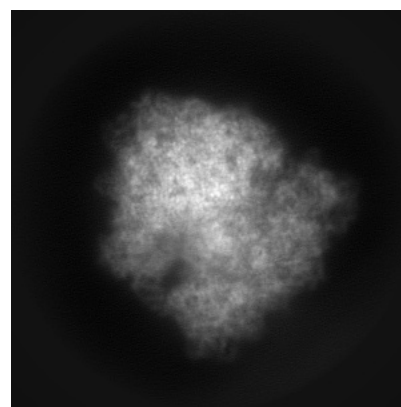
6.1.2 Raw map



X



Y

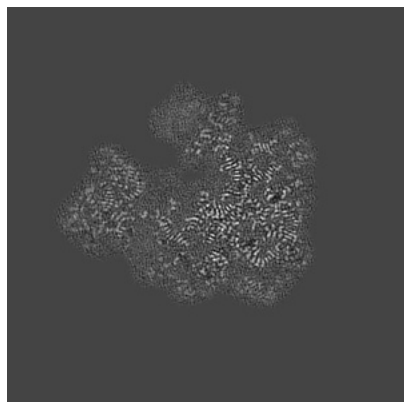


Z

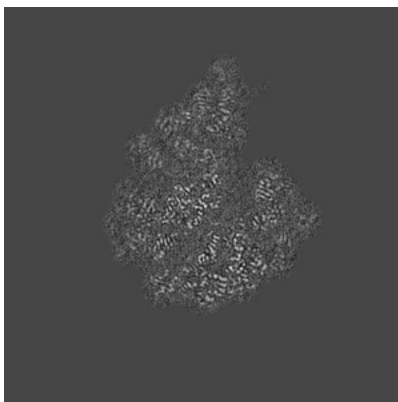
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

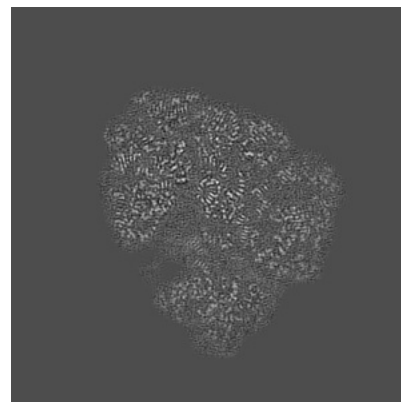
6.2.1 Primary map



X Index: 180

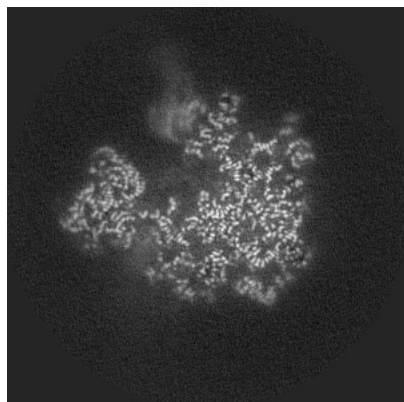


Y Index: 180

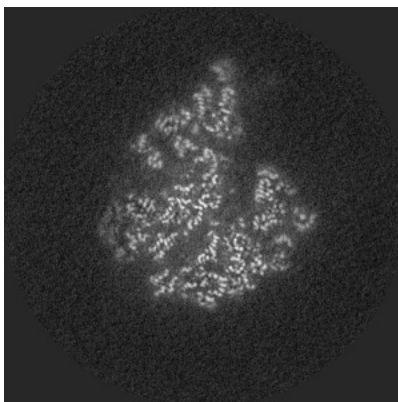


Z Index: 180

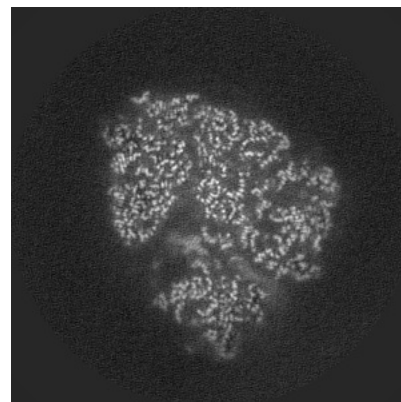
6.2.2 Raw map



X Index: 180



Y Index: 180

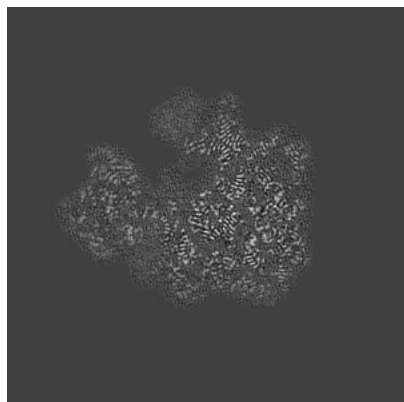


Z Index: 180

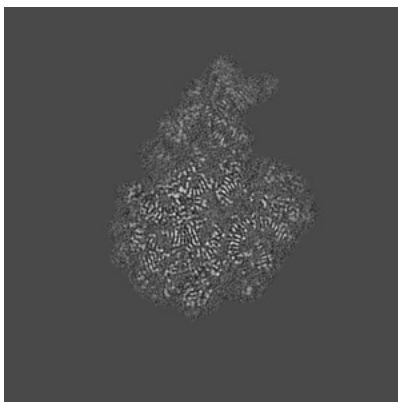
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

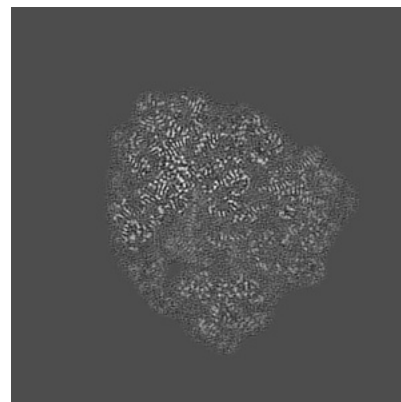
6.3.1 Primary map



X Index: 185

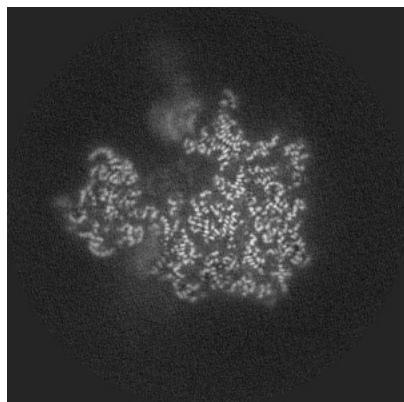


Y Index: 190

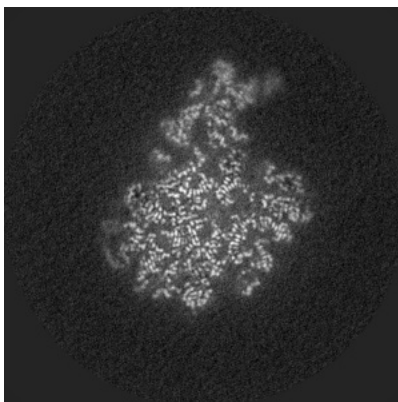


Z Index: 187

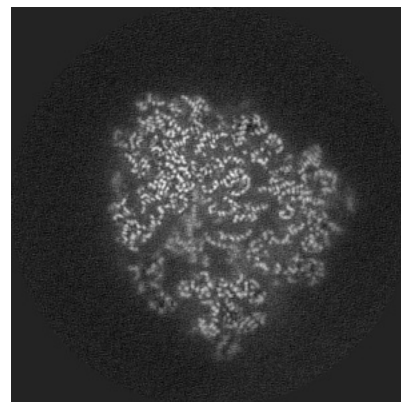
6.3.2 Raw map



X Index: 185



Y Index: 190

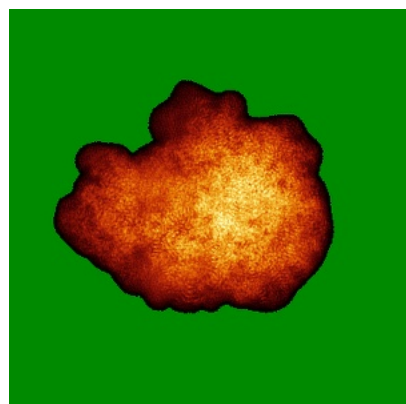


Z Index: 187

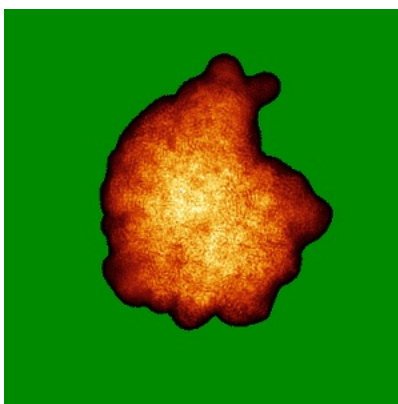
The images above show the largest variance slices of the map in three orthogonal directions.

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

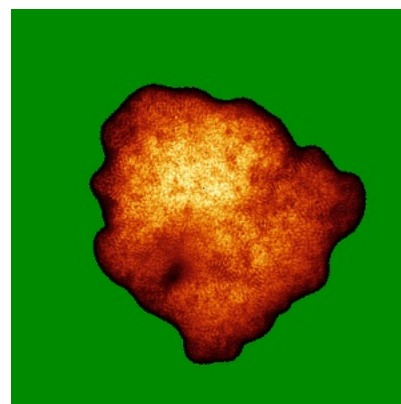
6.4.1 Primary map



X

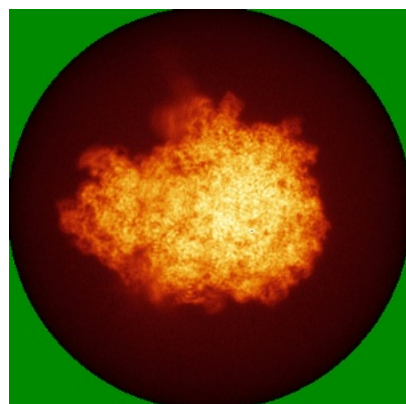


Y

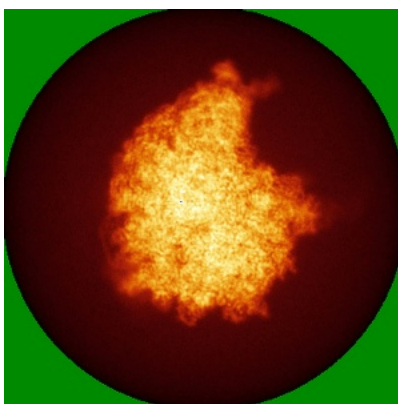


Z

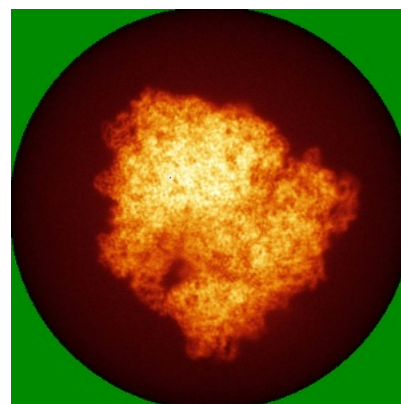
6.4.2 Raw map



X



Y

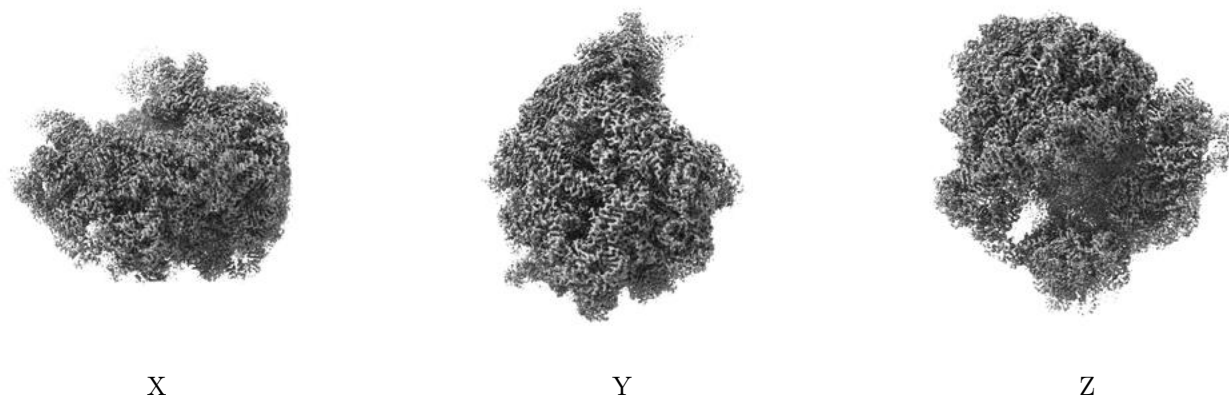


Z

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

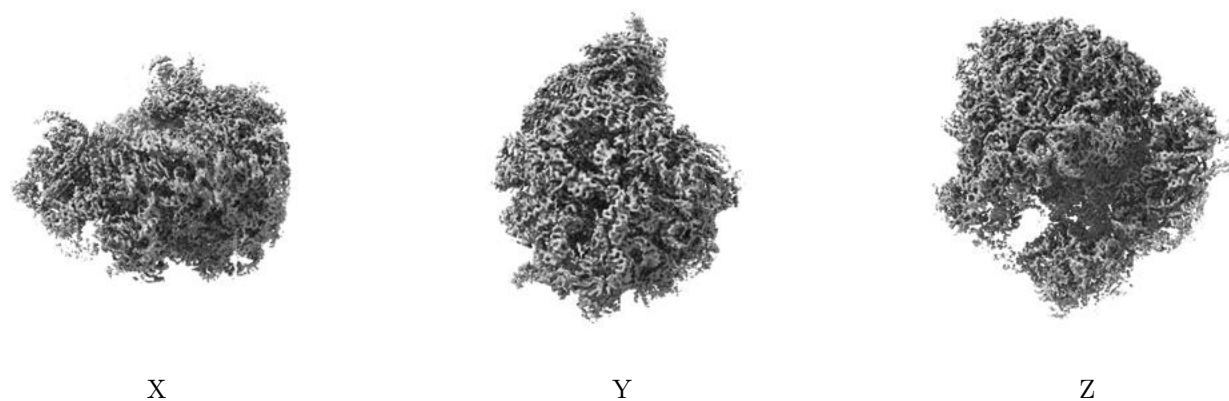
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

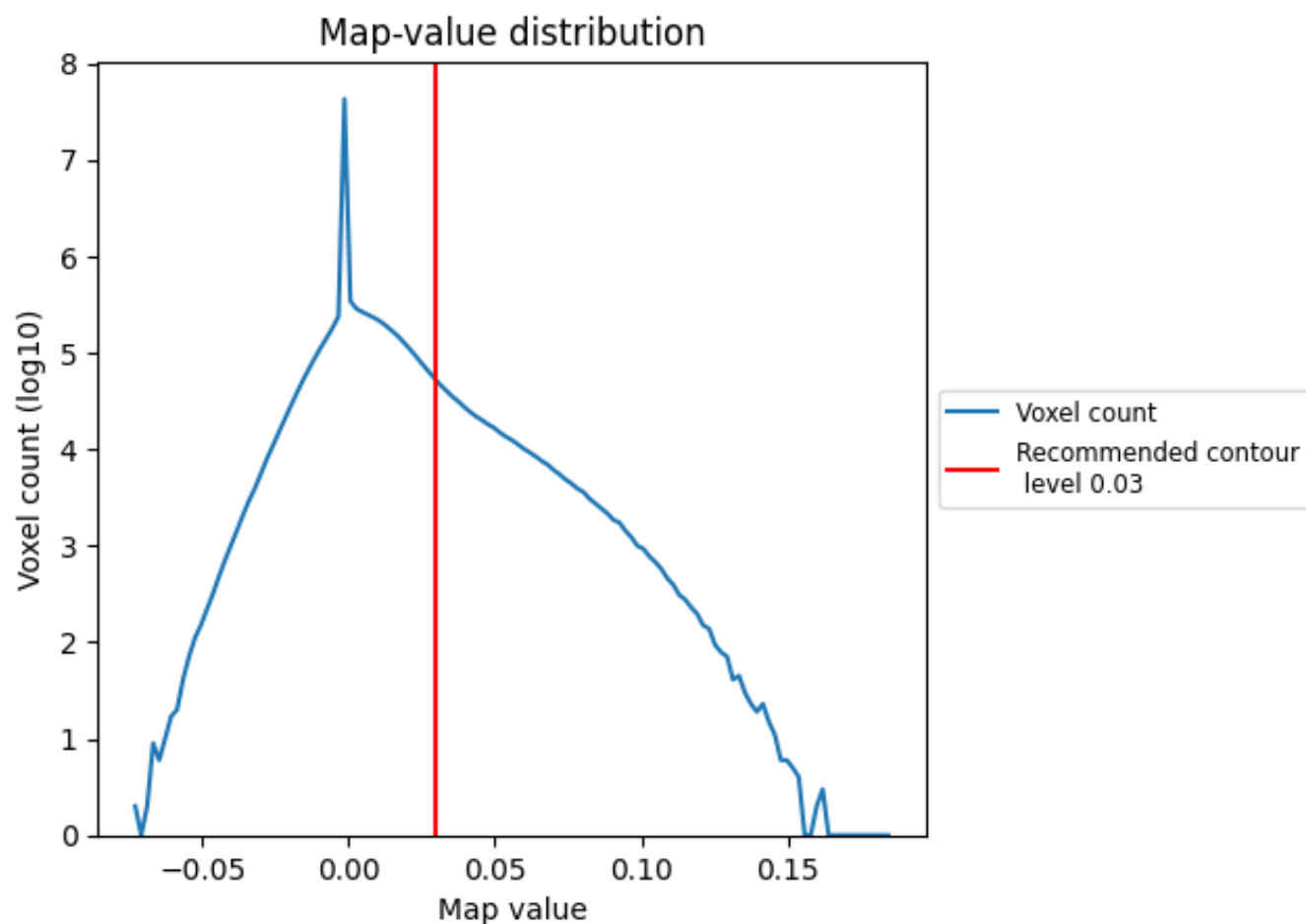
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

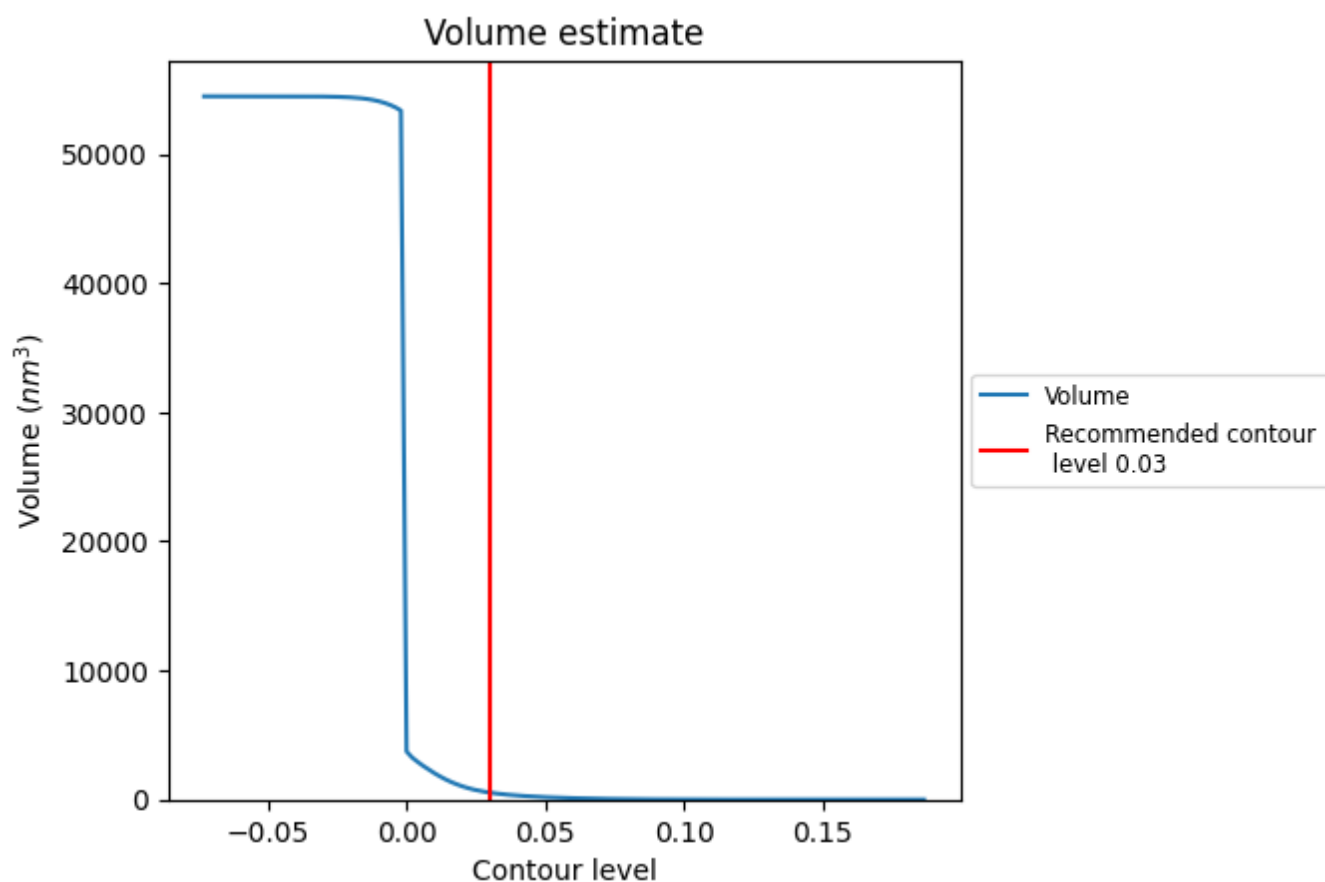
This section contains the results of statistical analysis of the map.

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.

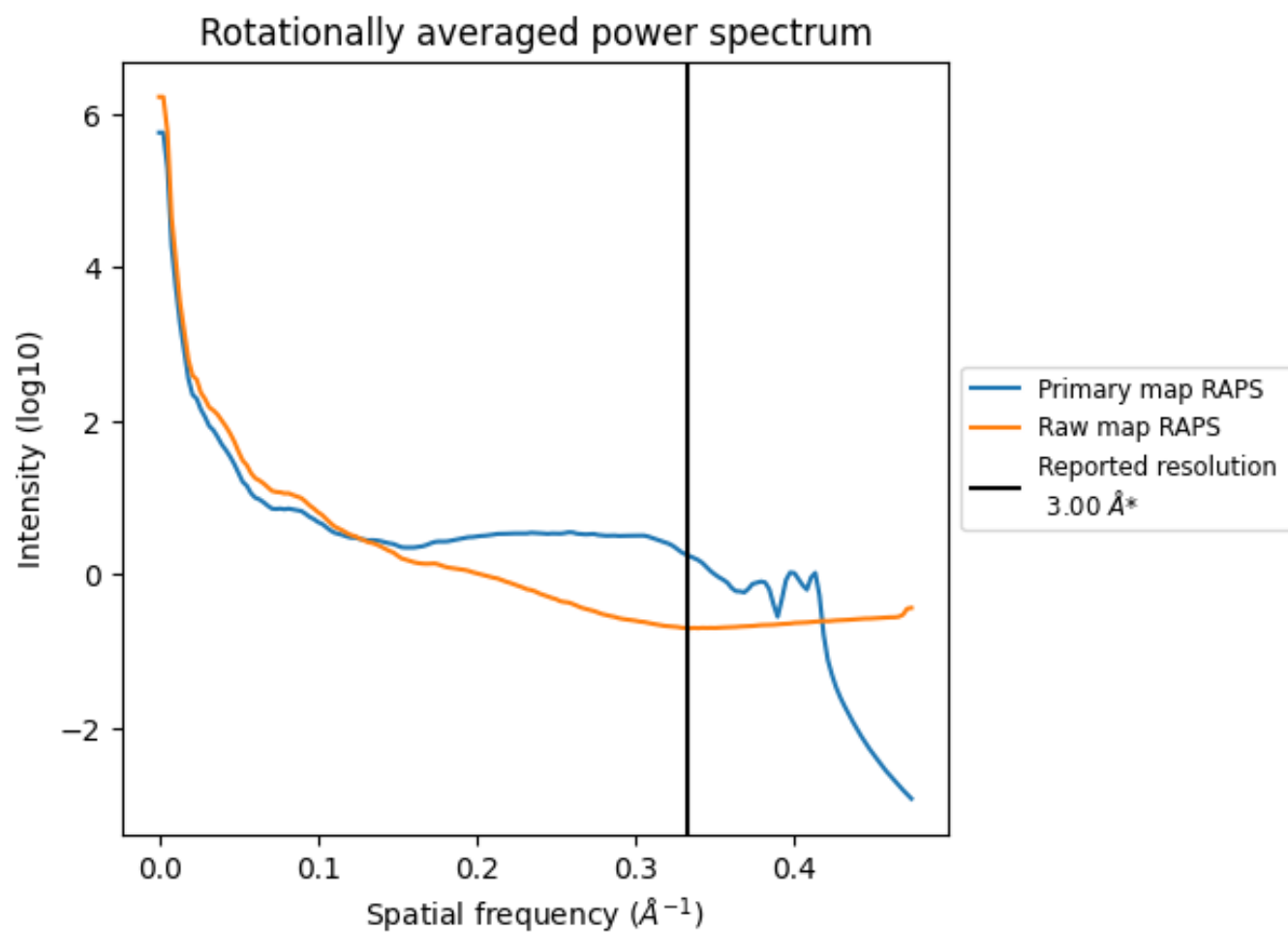
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 541 nm^3 ; this corresponds to an approximate mass of 489 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 ⓘ

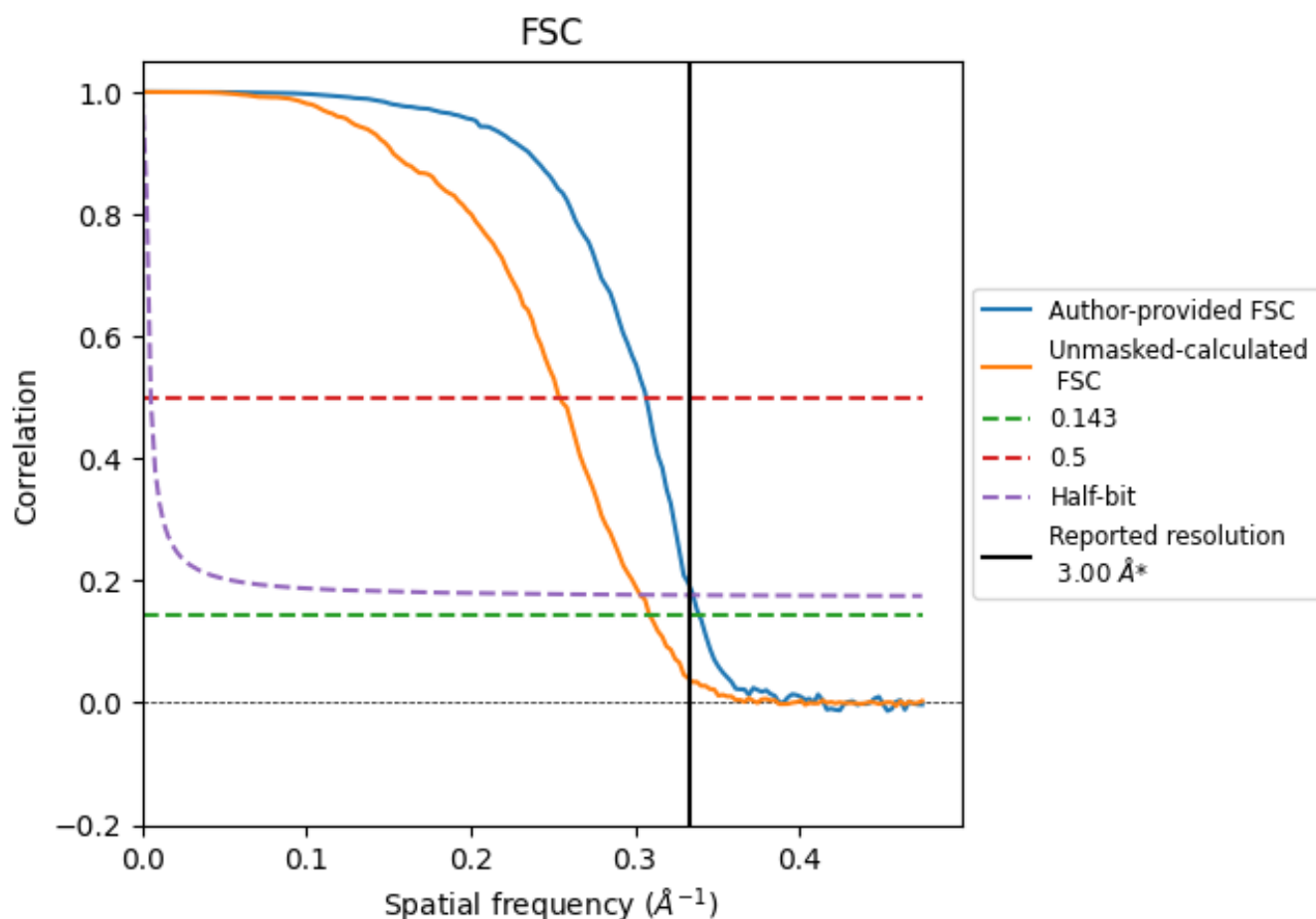


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.95	3.26	2.98
Unmasked-calculated*	3.24	3.93	3.30

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

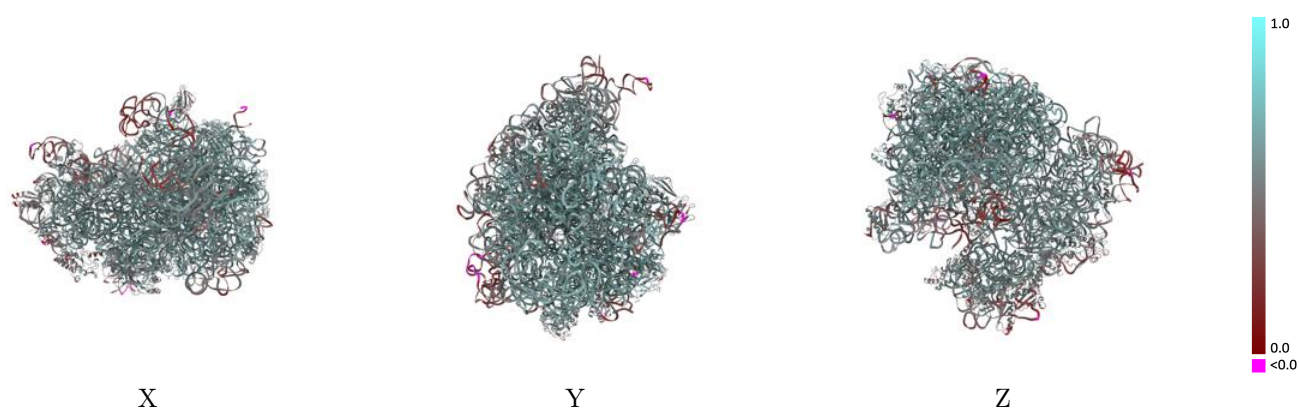
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15905 and PDB model 8B7Y. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

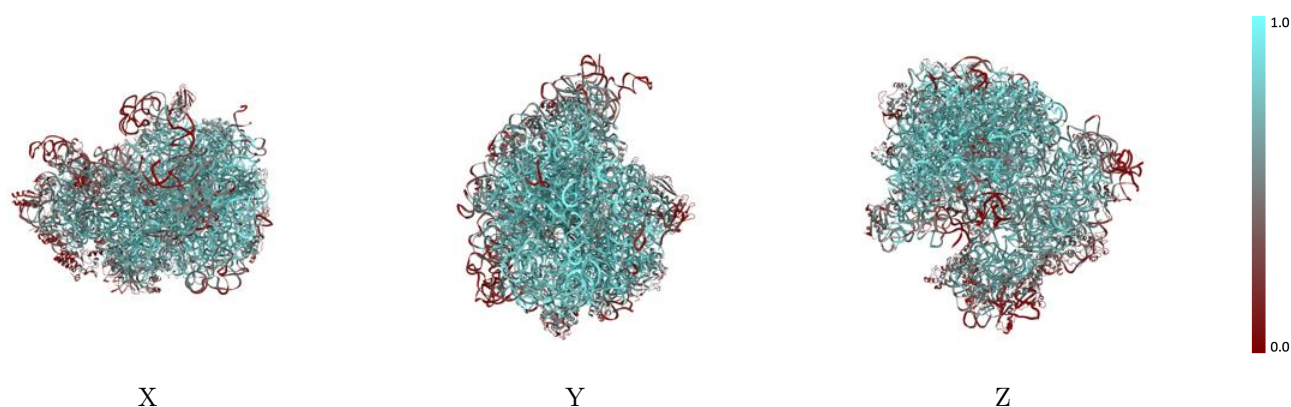
This section was not generated.

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



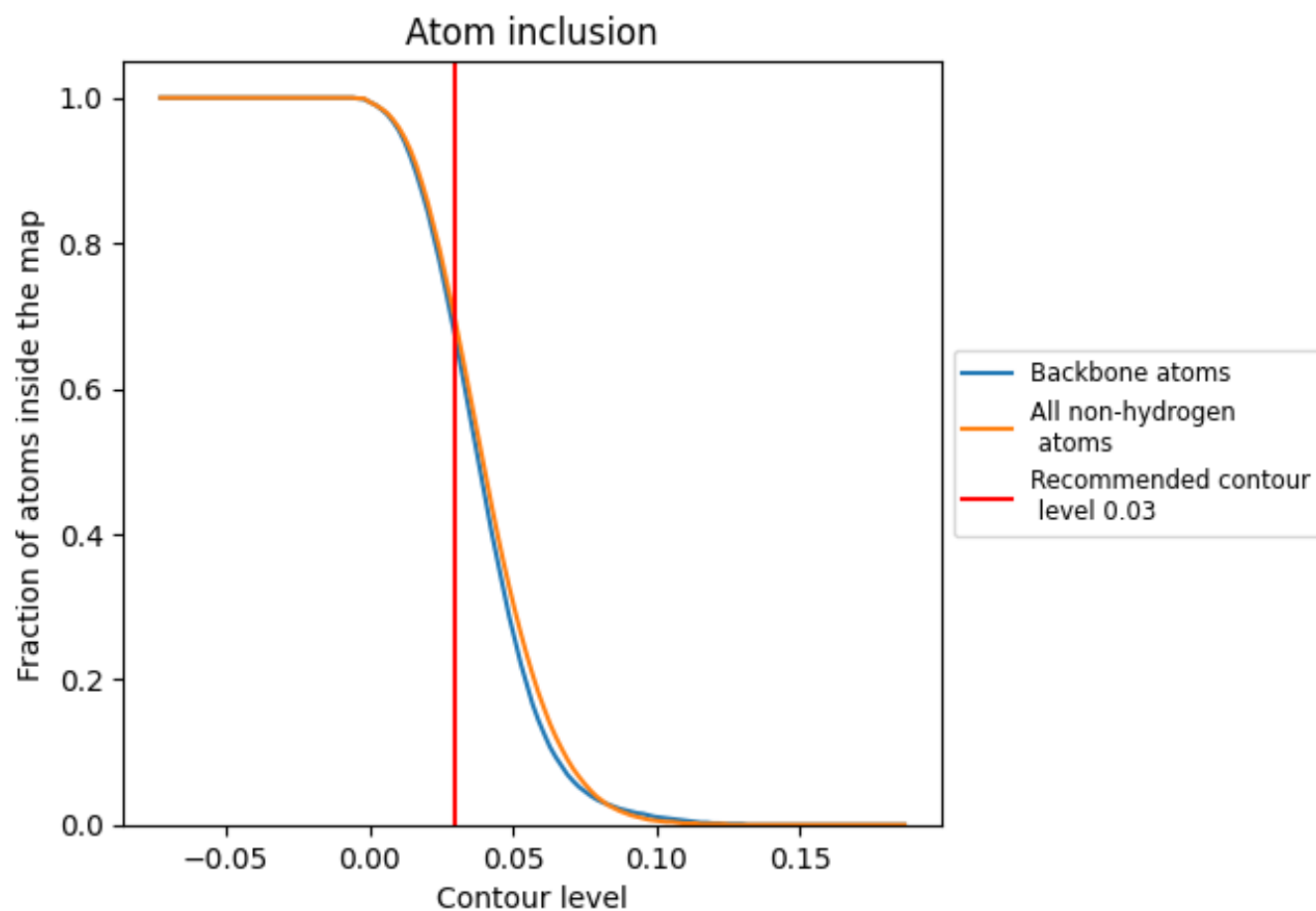
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 69% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6910	 0.5560
5	 0.2770	 0.4380
6	 0.8790	 0.6100
C	 0.6960	 0.5480
D	 0.2600	 0.4510
E	 0.4970	 0.5310
F	 0.3200	 0.4650
G	 0.6300	 0.5760
H	 0.4230	 0.5020
I	 0.7900	 0.5740
J	 0.6270	 0.5090
K	 0.7990	 0.6130
L	 0.7080	 0.5960
M	 0.5820	 0.5510
N	 0.2950	 0.4570
O	 0.3550	 0.4890
P	 0.5920	 0.5580
Q	 0.3820	 0.4980
R	 0.7140	 0.5870
S	 0.7230	 0.5940
T	 0.6670	 0.5770
U	 0.7220	 0.5910
V	 0.7760	 0.6050
W	 0.4960	 0.5320
X	 0.6810	 0.5790
Y	 0.7740	 0.6080
Z	 0.5760	 0.5520
a	 0.7090	 0.5810
b	 0.5940	 0.5470
c	 0.4210	 0.5000
d	 0.5400	 0.5510
e	 0.7710	 0.6110
f	 0.6940	 0.5890
g	 0.4190	 0.4980
h	 0.6440	 0.5770



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Chain	Atom inclusion	Q-score
i	 0.6990	 0.5850
j	 0.5460	 0.5520
k	 0.8510	 0.6130
l	 0.8370	 0.6190
m	 0.7440	 0.5950
n	 0.4510	 0.4590
o	 0.3390	 0.4630
p	 0.5180	 0.5260
q	 0.5750	 0.5490
r	 0.4100	 0.5070
s	 0.5080	 0.5270
t	 0.5770	 0.5480
u	 0.4460	 0.5160
v	 0.4620	 0.5160
w	 0.5560	 0.5410
x	 0.3830	 0.4910
y	 0.4470	 0.5050
z	 0.8320	 0.6240