



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 10:21 AM UTC

PDB ID : 9B1X / pdb_00009b1x
EMDB ID : EMD-44091
Title : HWS19 strain gidB mutant mycobacterial ribosome
Authors : Chen, Y.; Young, I.D.; Fraser, J.S.; Javid, B.
Deposited on : 2024-03-14
Resolution : 3.07 Å (reported)
Based on initial models : 5o60, 5o5j

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:

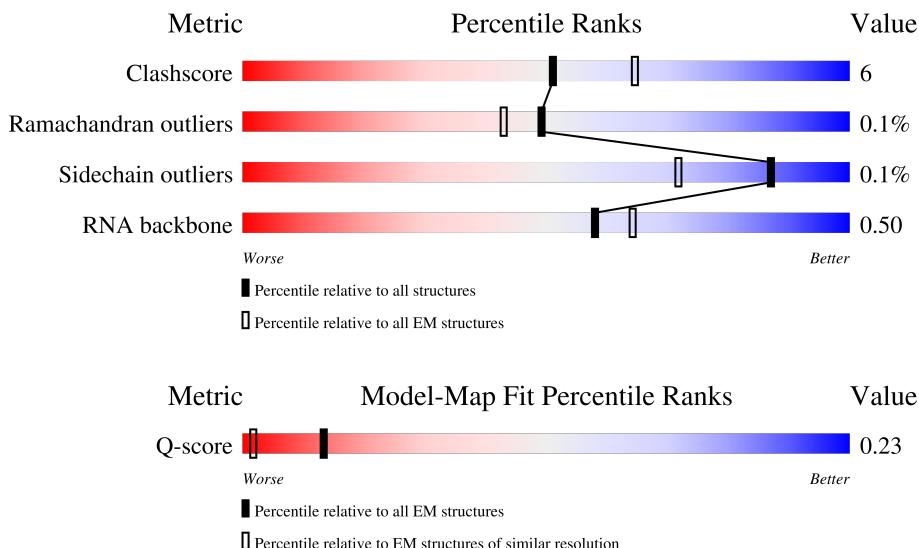
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.07 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	13977 (2.57 - 3.57)

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	A	1528	
2	B	33	
3	C	275	

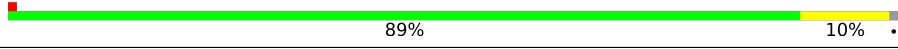
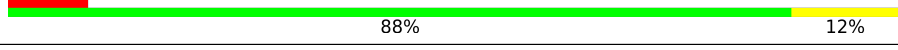
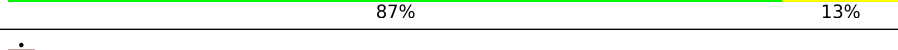
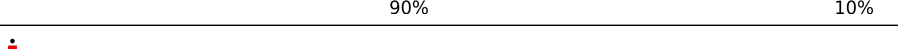
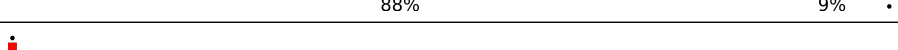
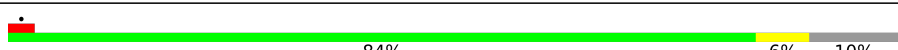
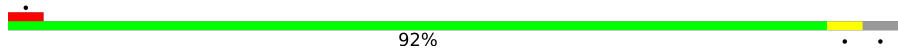
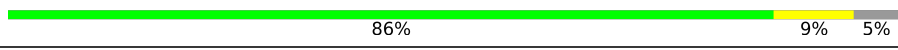
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Mol	Chain	Length	Quality of chain
4	D	201	
5	E	214	
6	F	96	
7	G	156	
8	H	132	
9	I	150	
10	J	101	
11	K	138	
12	L	124	
13	M	124	
14	N	61	
15	O	89	
16	P	156	
17	Q	98	
18	R	84	
19	S	93	
20	T	86	
21	V	277	
22	X	6	
23	Y	3120	
24	U	118	
25	Z	278	
26	a	217	
27	b	215	
28	c	187	

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Mol	Chain	Length	Quality of chain
29	d	179	
30	e	142	
31	f	147	
32	g	122	
33	h	147	
34	i	138	
35	j	199	
36	k	127	
37	l	113	
38	m	129	
39	n	103	
40	o	153	
41	p	100	
42	q	105	
43	r	215	
44	s	88	
45	t	64	
46	u	77	
47	5	24	
48	v	175	
49	w	61	
50	x	57	
51	y	55	
52	z	47	
53	1	64	

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Mol	Chain	Length	Quality of chain
54	2	37	5% 86% 14%

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 242013 atoms, of which 97195 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 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1511	Total	C	H	N	O	P	0	0
			48755	14448	16316	5930	10550	1511		

- Molecule 2 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	32	Total	C	H	N	O	S	0	0
			623	172	343	71	36	1		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	208	Total	C	H	N	O	S	0	0
			3368	1036	1708	322	298	4		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	200	Total	C	H	N	O	S	0	0
			3310	1028	1669	316	295	2		

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	180	Total	C	H	N	O	S	0	0
			2657	812	1361	245	235	4		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	96	Total	C	H	N	O	S	0	0
			1568	486	797	138	145	2		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	155	Total	C	H	N	O	S	0	0
			2514	768	1282	241	221	2		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	131	Total	C	H	N	O	S	0	0
			2057	633	1047	189	187	1		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	126	Total	C	H	N	O	S	0	0
			2044	630	1050	194	170			

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	99	Total	C	H	N	O	S	0	0
			1608	495	820	146	144	3		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1719	528	864	170	156	1		

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	122	Total	C	H	N	O	S	0	0
			2003	594	1045	197	165	2		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	116	Total	C	H	N	O	S	0	0
			1922	572	987	191	169	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	60	Total	C	H	N	O	S	0	0
			981	302	504	97	73	5		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	88	Total	C	H	N	O		0	0
			1481	449	761	147	124			

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	113	Total	C	H	N	O		0	0
			1827	570	936	162	159			

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	94	Total	C	H	N	O	S	0	0
			1544	469	796	142	135	2		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18B.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	65	Total	C	H	N	O	S	0	0
			1054	318	541	102	90	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	82	Total	C	H	N	O	S	0	0
			1339	425	677	124	112	1		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	85	Total	C	H	N	O		0	0
			1373	402	713	139	119			

- Molecule 21 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	V	228	Total	C	H	N	O	S	0	0
			3632	1132	1839	322	330	9		

- Molecule 22 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	X	6	Total	C	H	N	O	P	0	0
			180	54	63	13	45	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Y	2954	Total	C	H	N	O	P	0	0
			95352	28279	31908	11682	20529	2954		

- Molecule 24 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	U	118	Total	C	H	N	O	P	0	0
			3807	1126	1285	468	810	118		

- Molecule 25 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	275	Total	C	H	N	O	S	0	0
			4276	1298	2166	438	370	4		

- Molecule 26 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	a	214	Total	C	H	N	O	S	0	0
			3218	982	1631	310	290	5		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	b	209	Total	C	H	N	O	S	0	0
			3177	969	1608	295	303	2		

- Molecule 28 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	c	182	Total	C	H	N	O	S	0	0
			2922	907	1477	271	261	6		

- Molecule 29 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	d	176	Total	C	H	N	O	S	0	0
			2748	845	1400	249	253	1		

- Molecule 30 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	e	133	Total	C	H	N	O	S	0	0
			2012	625	1022	175	187	3		

- Molecule 31 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	f	146	Total	C	H	N	O	S	0	0
			2297	722	1167	207	200	1		

- Molecule 32 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	g	122	Total	C	H	N	O	S	0	0
			1938	586	1000	179	170	3		

- Molecule 33 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	h	145	Total	C	H	N	O	S	0	0
			2230	676	1152	205	194	3		

- Molecule 34 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	i	136	Total	C	H	N	O	S	0	0
			2220	690	1128	213	187	2		

- Molecule 35 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	j	118	Total	C	H	N	O	S	0	0
			1900	583	972	180	163	2		

- Molecule 36 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	k	126	Total	C	H	N	O		0	0
			1948	586	992	199	171			

- Molecule 37 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	l	113	Total	C	H	N	O	S	0	0
			1845	570	938	171	165	1		

- Molecule 38 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	m	124	Total	C	H	N	O		0	0
			2027	613	1039	203	172			

- Molecule 39 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	n	100	Total	C	H	N	O		0	0
			1557	478	803	137	139			

- Molecule 40 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	o	114	Total	C	H	N	O		0	0
			1783	543	910	171	159			

- Molecule 41 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	p	97	Total	C	H	N	O		0	0
			1559	479	803	138	139			

- Molecule 42 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	q	97	Total	C	H	N	O	S	0	0
			1515	456	783	137	137	2		

- Molecule 43 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	r	192	Total	C	H	N	O		0	0
			2872	881	1444	255	292			

- Molecule 44 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	s	79	Total	C	H	N	O		0	0
			1188	361	602	123	102			

- Molecule 45 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	t	63	Total	C	H	N	O	S	0	0
			955	283	485	103	80	4		

- Molecule 46 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	u	64	Total	C	H	N	O	S	0	0
			1073	324	542	103	103	1		

- Molecule 47 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	5	23	Total	C	H	N	O		0	0
			395	111	206	50	28			

- Molecule 48 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	v	126	Total	C	H	N	O	S	0	0
			1877	580	959	156	180	2		

- Molecule 49 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	59	Total	C	H	N	O	0	0
			975	292	501	95	87		

- Molecule 50 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	54	Total	C	H	N	O S	0	0
			887	260	464	93	69 1		

- Molecule 51 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	49	Total	C	H	N	O S	0	0
			817	248	412	82	71 4		

- Molecule 52 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	46	Total	C	H	N	O S	0	0
			789	225	412	97	54 1		

- Molecule 53 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	63	Total	C	H	N	O	0	0
			1043	302	541	115	85		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	37	Total	C	H	N	O S	0	0
			623	181	324	66	47 5		

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

Mol	Chain	Residues	Atoms		AltConf
55	A	212	Total	Mg	0
			212	212	
55	B	1	Total	Mg	0
			1	1	
55	F	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
55	N	1	Total 1	Mg 1	0
55	P	1	Total 1	Mg 1	0
55	R	1	Total 1	Mg 1	0
55	Y	381	Total 381	Mg 381	0
55	U	9	Total 9	Mg 9	0
55	Z	9	Total 9	Mg 9	0
55	b	1	Total 1	Mg 1	0
55	c	1	Total 1	Mg 1	0
55	i	1	Total 1	Mg 1	0
55	o	1	Total 1	Mg 1	0
55	p	1	Total 1	Mg 1	0
55	s	1	Total 1	Mg 1	0
55	t	1	Total 1	Mg 1	0
55	1	1	Total 1	Mg 1	0

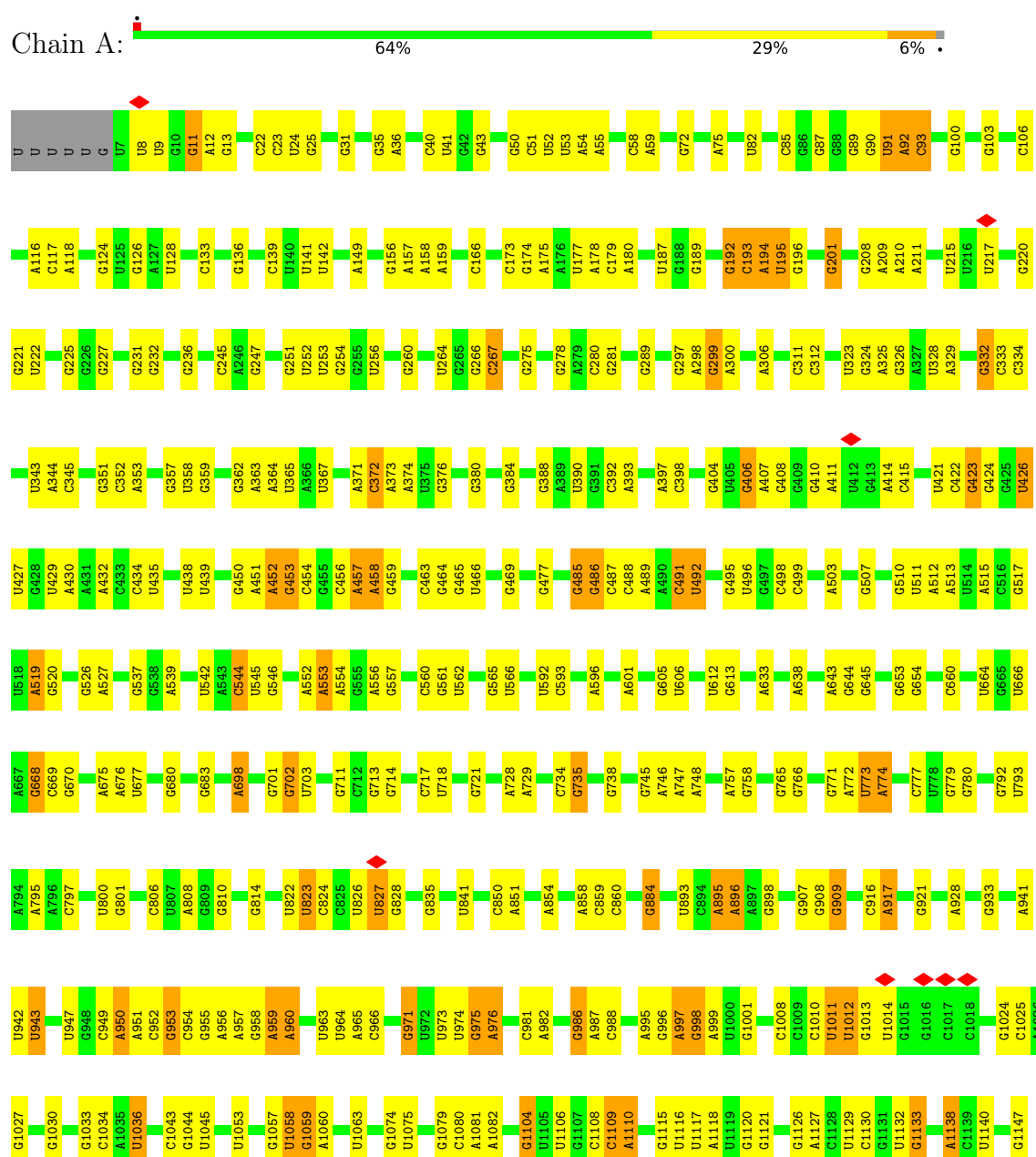
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

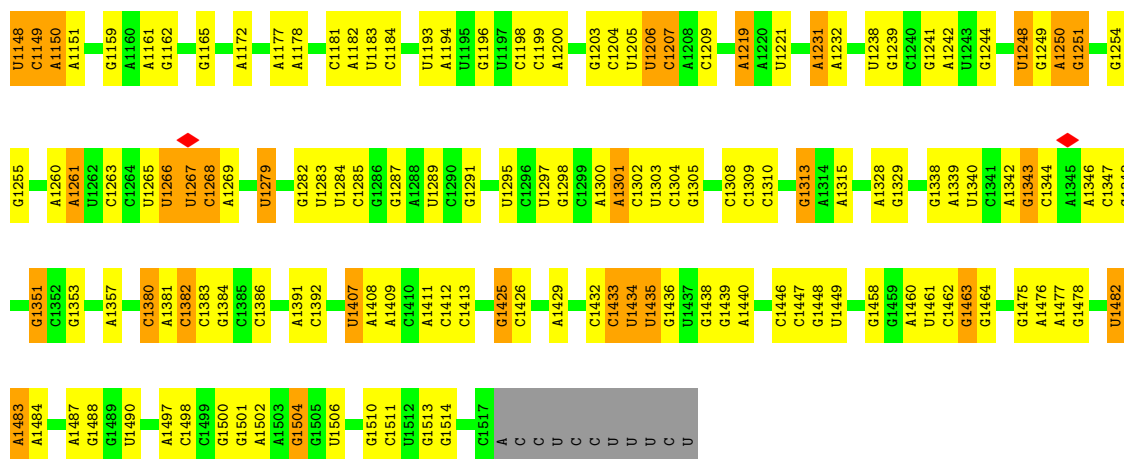
Mol	Chain	Residues	Atoms		AltConf
56	N	1	Total 1	Zn 1	0
56	R	1	Total 1	Zn 1	0
56	t	1	Total 1	Zn 1	0
56	y	1	Total 1	Zn 1	0
56	2	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

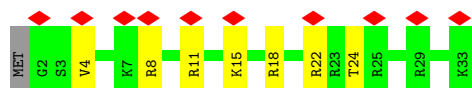
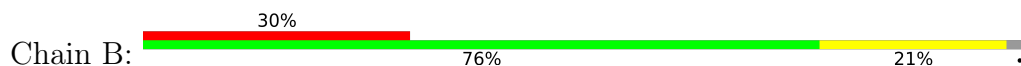
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

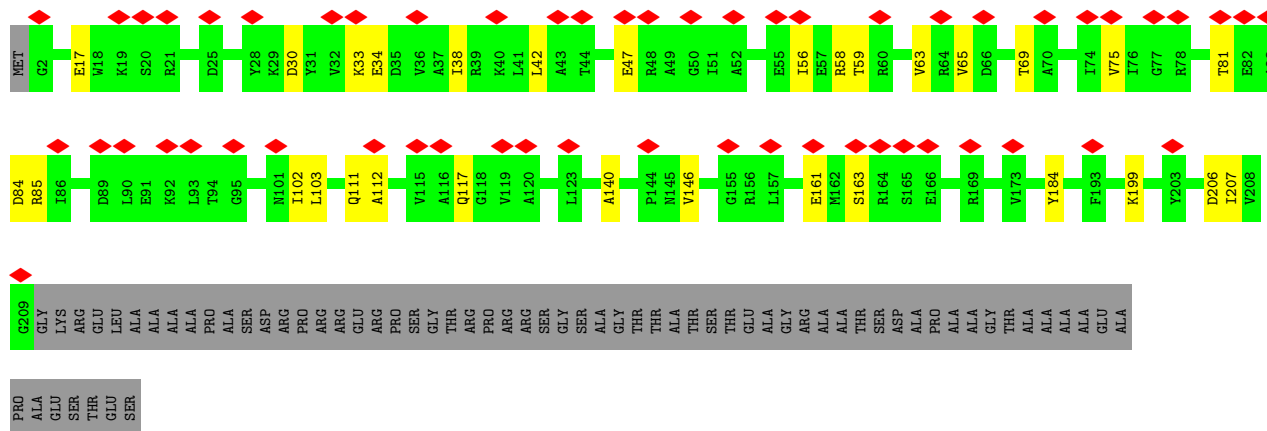




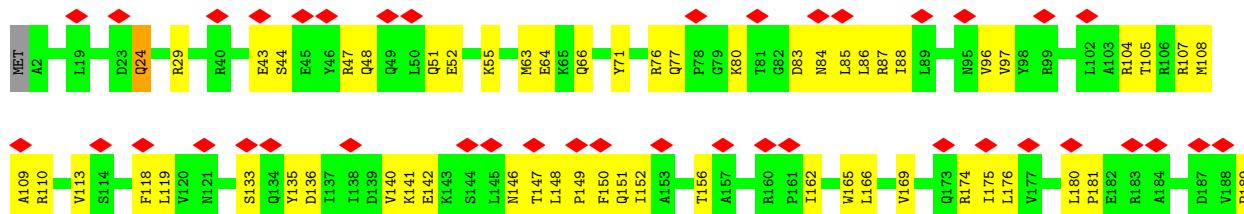
- Molecule 2: Conserved domain protein

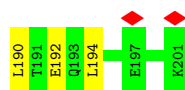


- Molecule 3: Small ribosomal subunit protein uS3

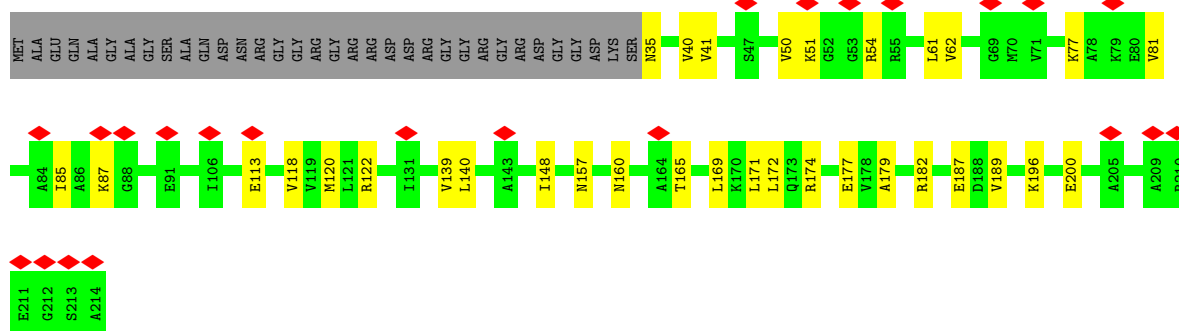


- Molecule 4: Small ribosomal subunit protein uS4

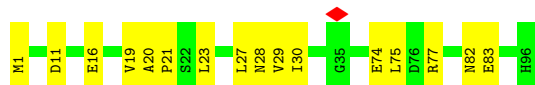
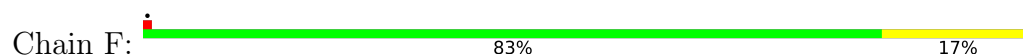




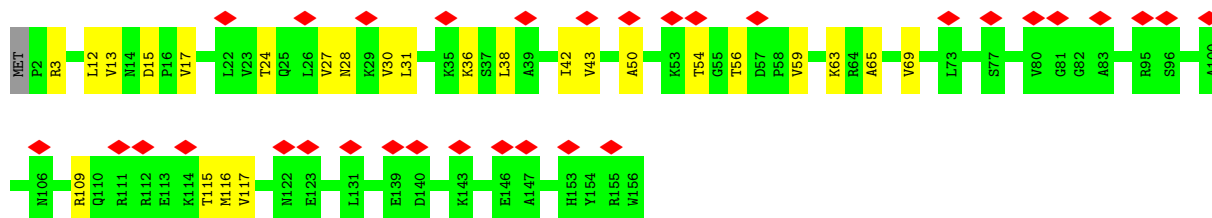
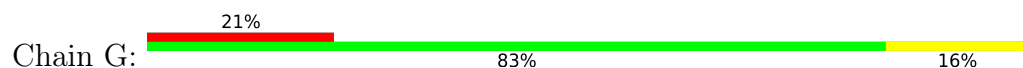
- Molecule 5: Small ribosomal subunit protein uS5



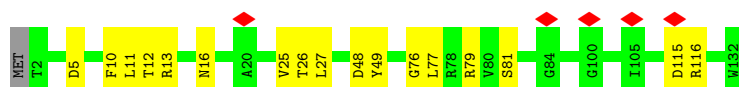
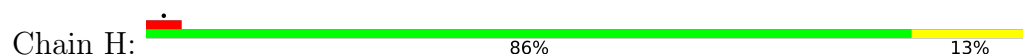
- Molecule 6: Small ribosomal subunit protein bS6



- Molecule 7: Small ribosomal subunit protein uS7

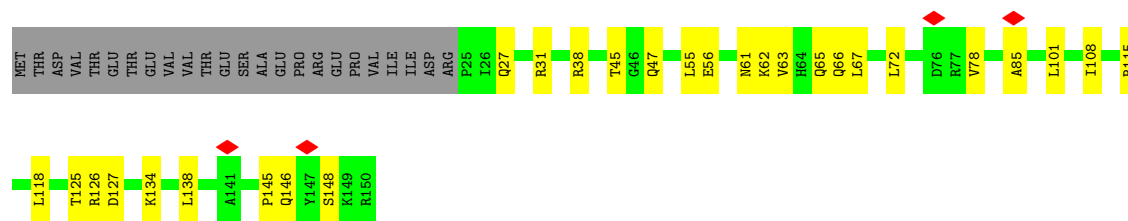


- Molecule 8: Small ribosomal subunit protein uS8

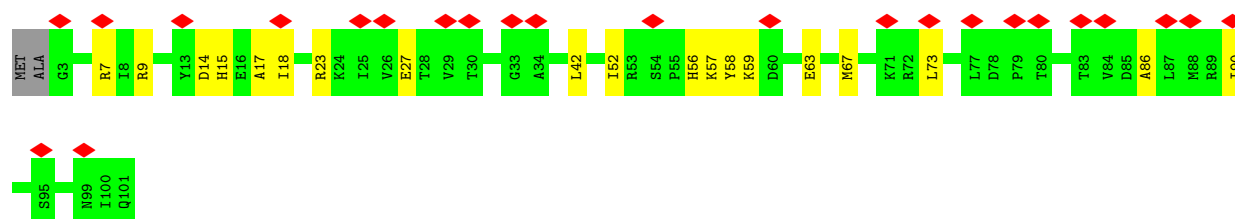
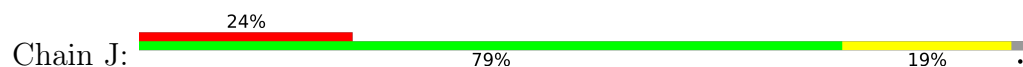


- Molecule 9: Small ribosomal subunit protein uS9

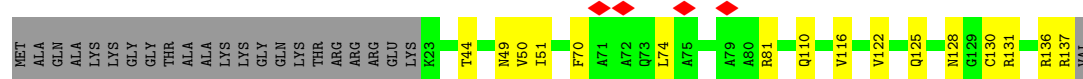




- Molecule 10: Small ribosomal subunit protein uS10



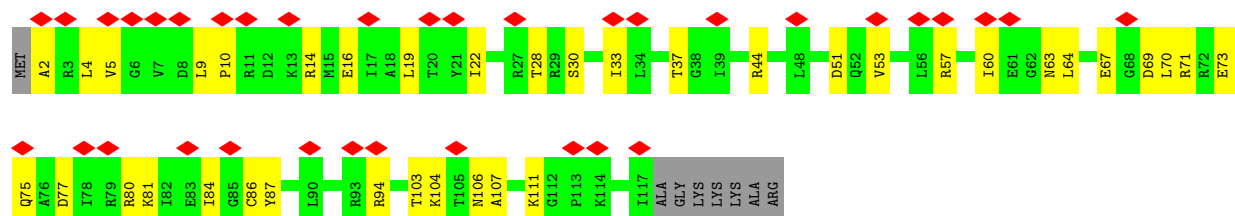
- Molecule 11: Small ribosomal subunit protein uS11



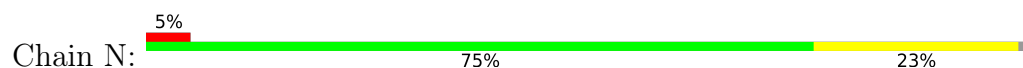
- Molecule 12: Small ribosomal subunit protein uS12



- Molecule 13: Small ribosomal subunit protein uS13

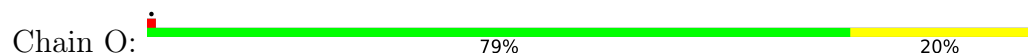


- Molecule 14: Small ribosomal subunit protein uS14B

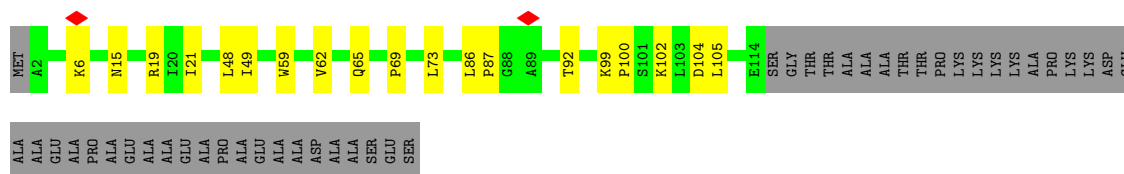




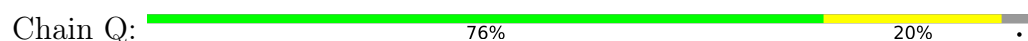
- Molecule 15: Small ribosomal subunit protein uS15



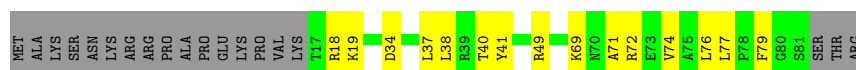
- Molecule 16: Small ribosomal subunit protein bS16



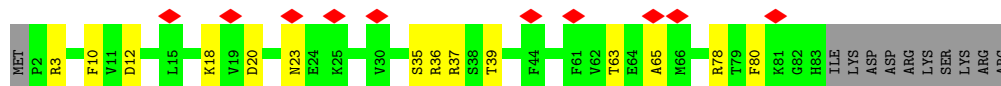
- Molecule 17: Small ribosomal subunit protein uS17



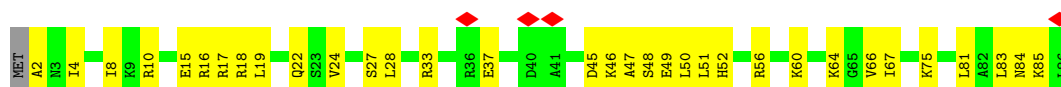
- Molecule 18: Small ribosomal subunit protein bS18B



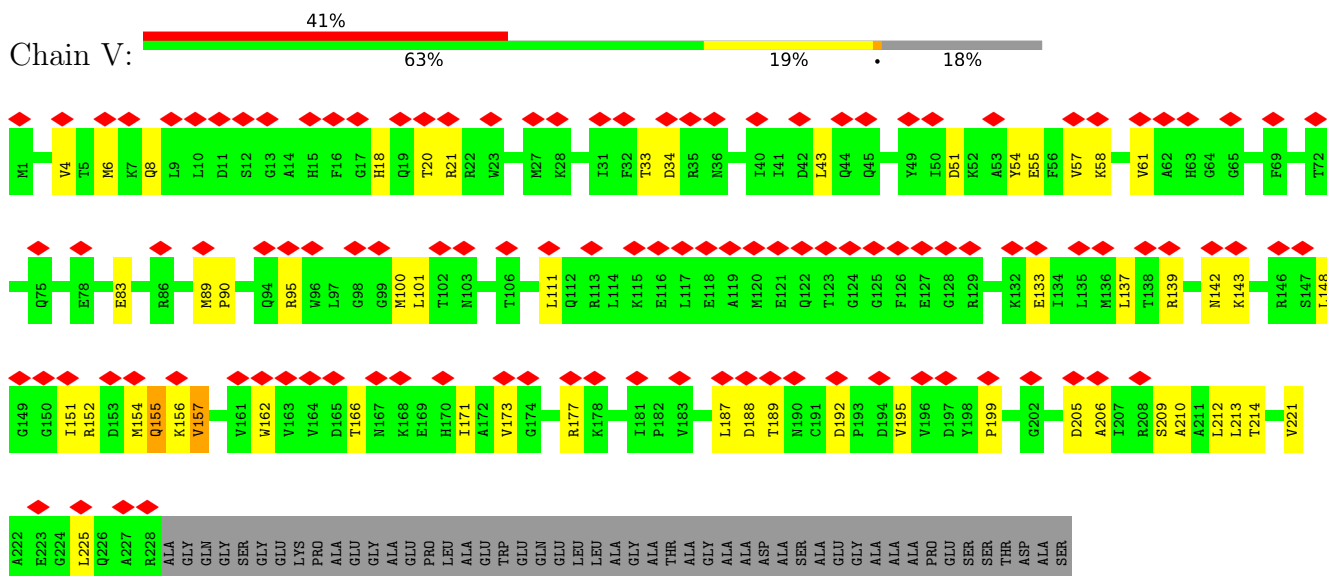
- Molecule 19: Small ribosomal subunit protein uS19



- Molecule 20: Small ribosomal subunit protein bS20



- Molecule 21: Small ribosomal subunit protein uS2

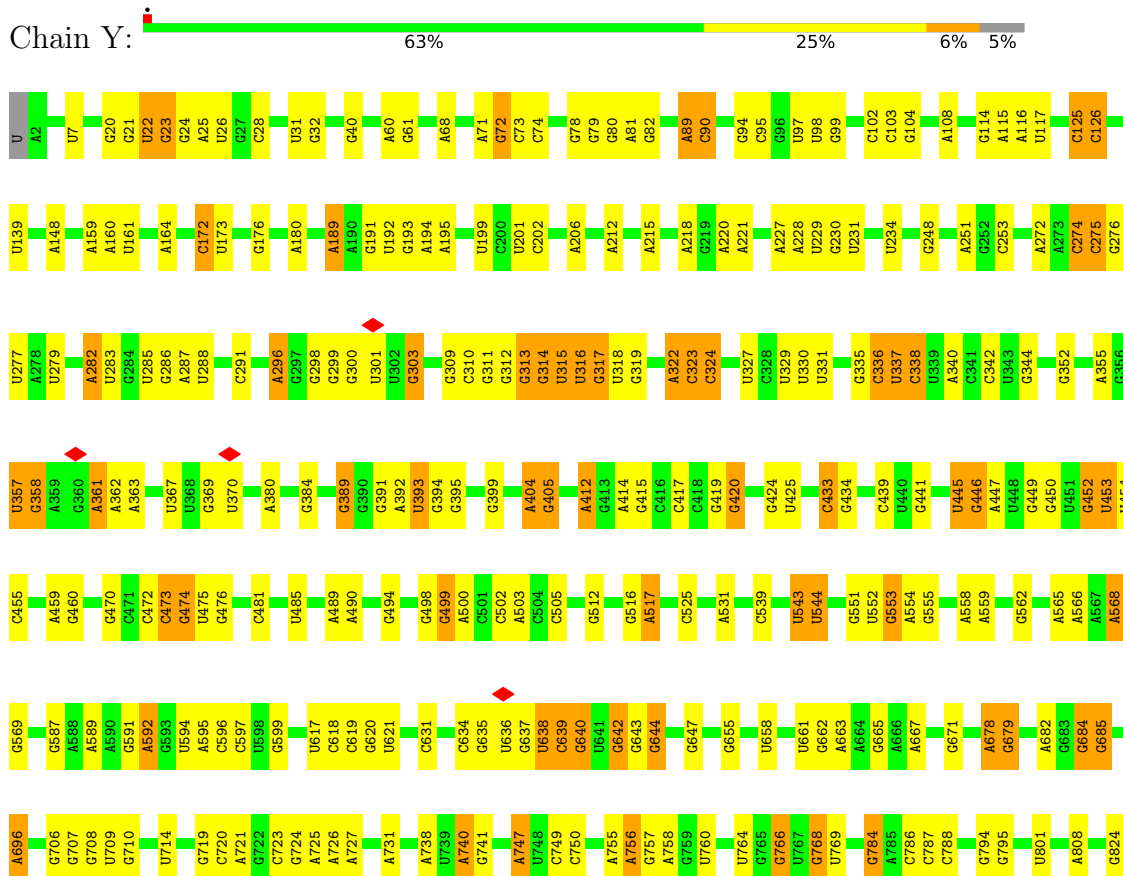


- Molecule 22: mRNA fragment

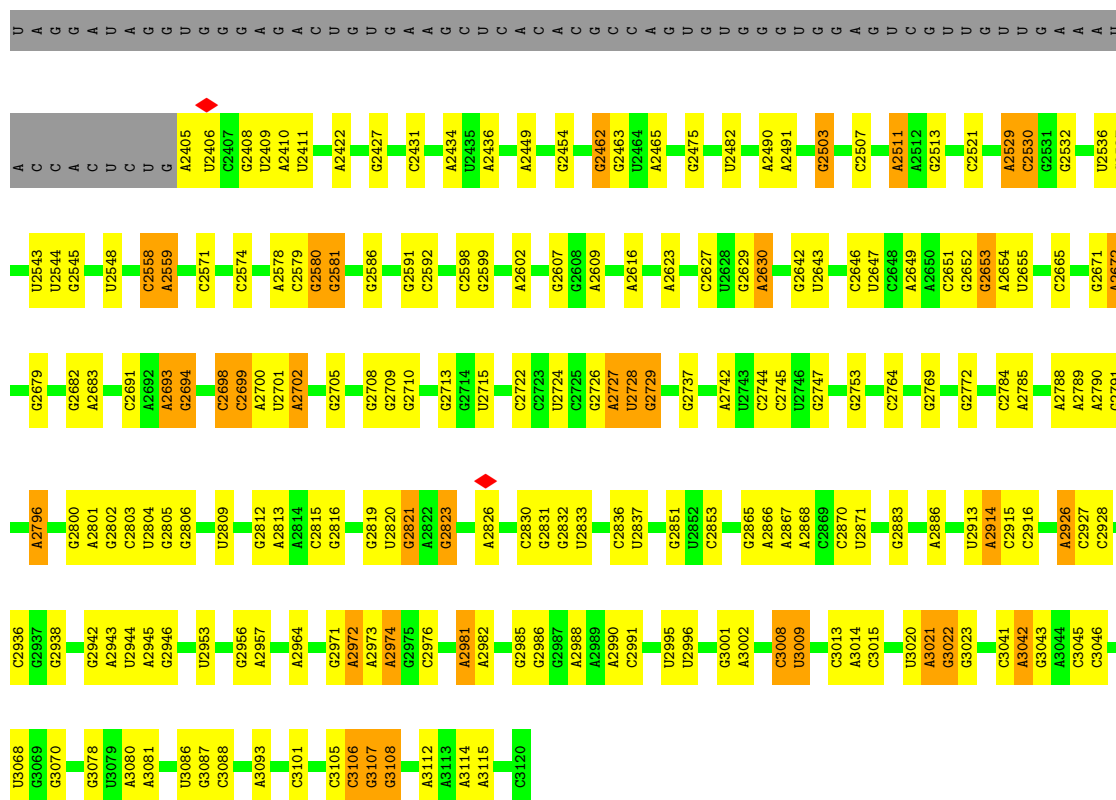


There are no outlier residues recorded for this chain.

- Molecule 23: 23S rRNA

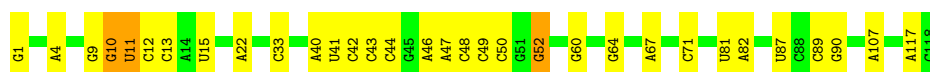






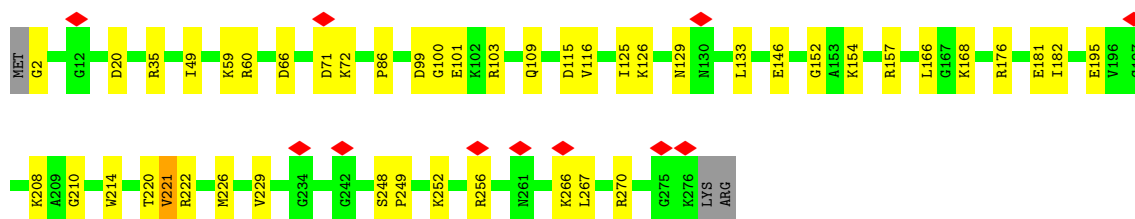
• Molecule 24: 5S rRNA

Chain U: 73% 25% .



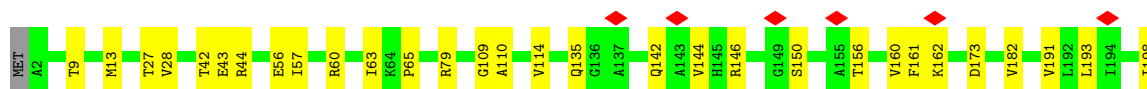
• Molecule 25: Large ribosomal subunit protein uL2

Chain Z: 82% 16% .



• Molecule 26: Large ribosomal subunit protein uL3

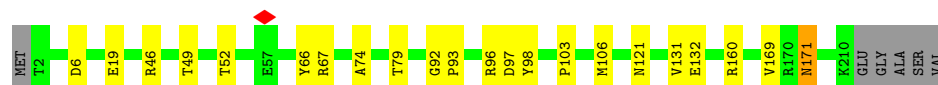
Chain a: 84% 15% .





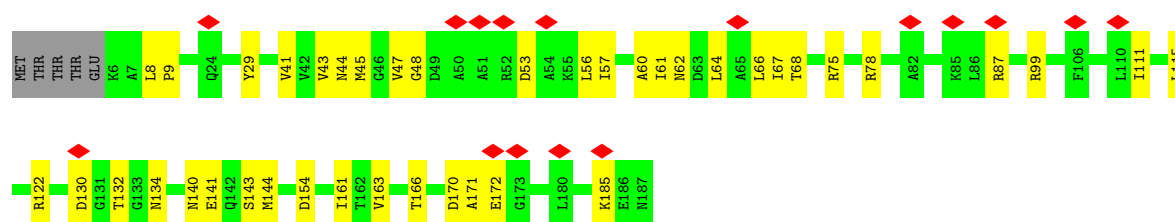
- Molecule 27: Large ribosomal subunit protein uL4

Chain b: 87% 10% .



- Molecule 28: Large ribosomal subunit protein uL5

Chain c: 9% 75% 22% .



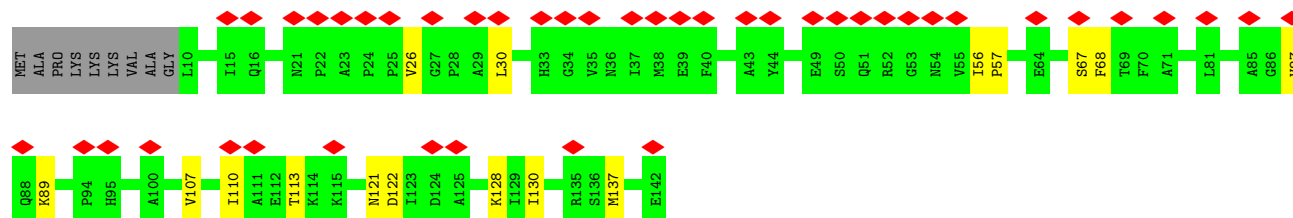
- Molecule 29: Large ribosomal subunit protein uL6

Chain d: 85% 13% .



- Molecule 30: Large ribosomal subunit protein uL11

Chain e: 31% 82% 11% 6% .

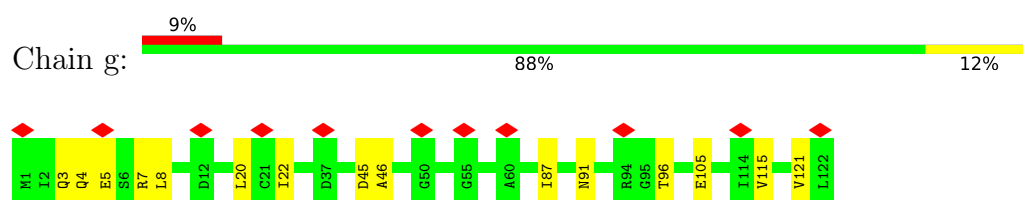


- Molecule 31: Large ribosomal subunit protein uL13

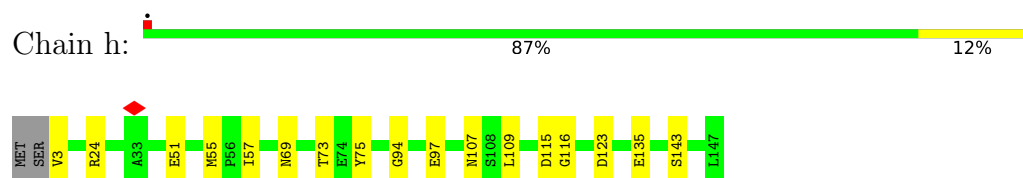
Chain f: 89% 10% .



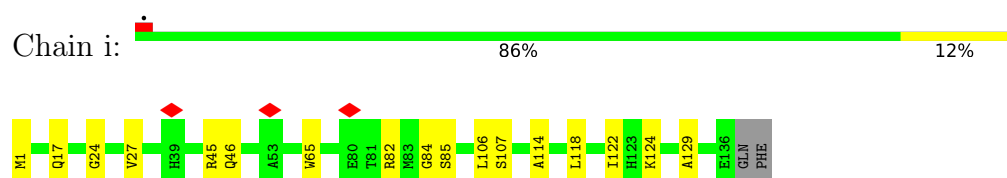
- Molecule 32: Large ribosomal subunit protein uL14



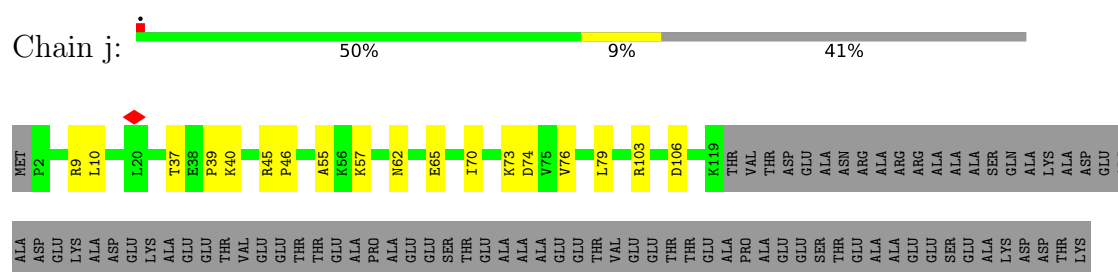
- Molecule 33: Large ribosomal subunit protein uL15



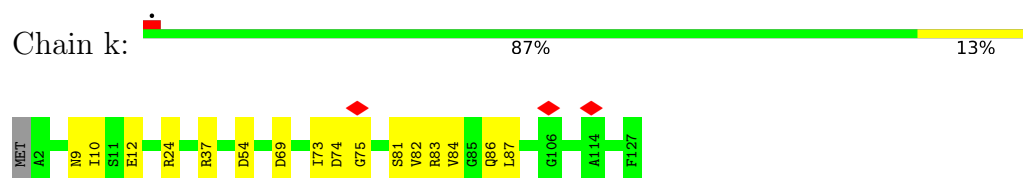
- Molecule 34: Large ribosomal subunit protein uL16



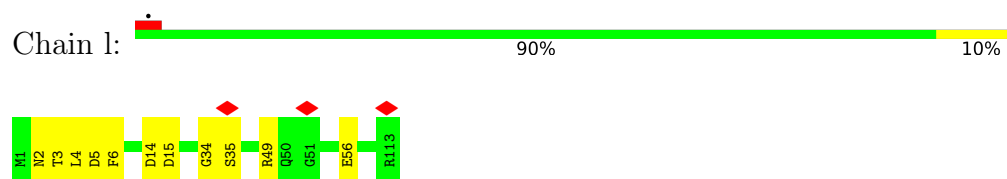
- Molecule 35: Large ribosomal subunit protein bL17



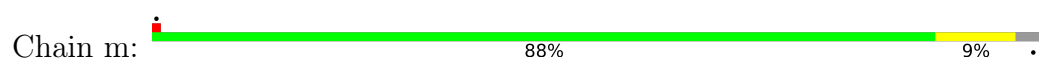
- Molecule 36: Large ribosomal subunit protein uL18



- Molecule 37: Large ribosomal subunit protein bL19

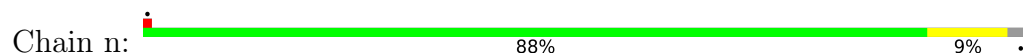


- Molecule 38: Large ribosomal subunit protein bL20

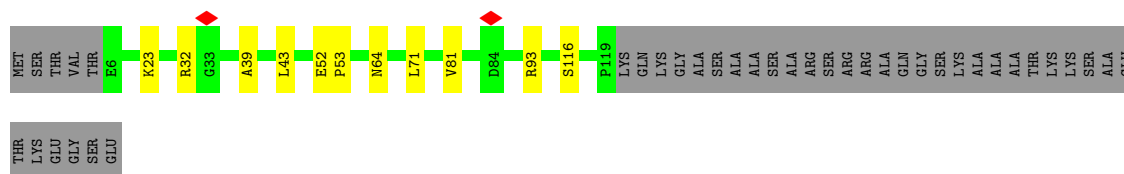




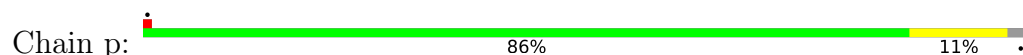
- Molecule 39: Large ribosomal subunit protein bL21



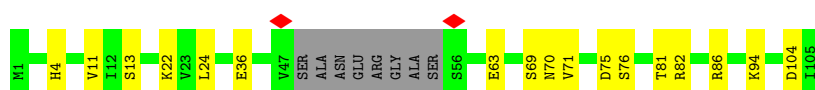
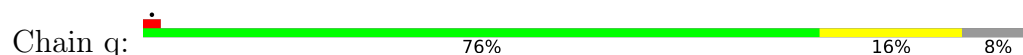
- Molecule 40: Large ribosomal subunit protein uL22



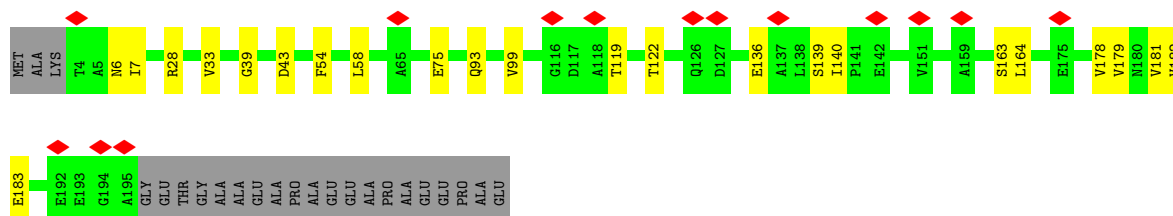
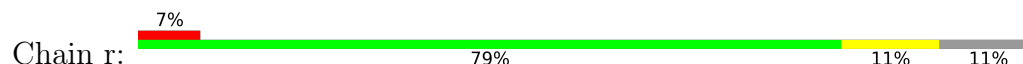
- Molecule 41: Large ribosomal subunit protein uL23



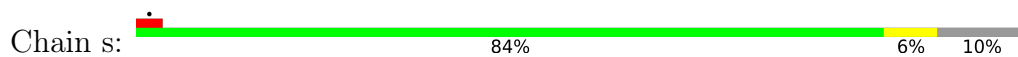
- Molecule 42: Large ribosomal subunit protein uL24



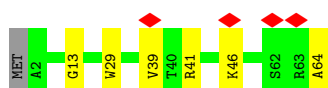
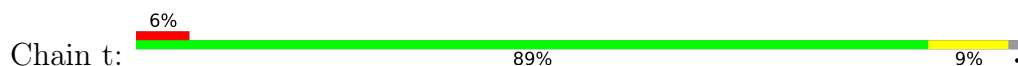
- Molecule 43: Large ribosomal subunit protein bL25



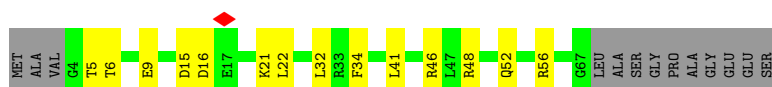
- Molecule 44: Large ribosomal subunit protein bL27



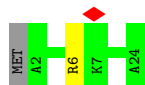
- Molecule 45: Large ribosomal subunit protein bL28



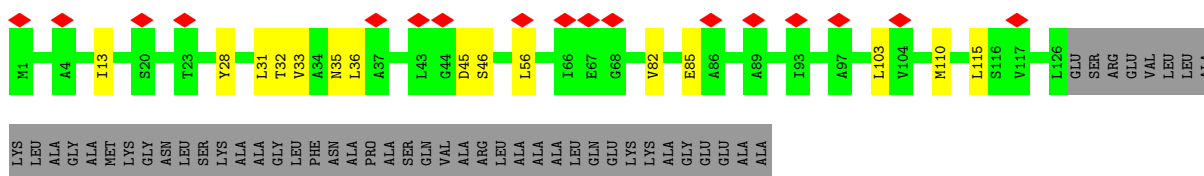
- Molecule 46: Large ribosomal subunit protein uL29



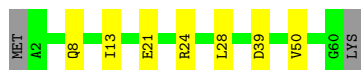
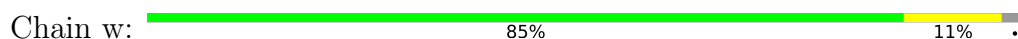
- Molecule 47: 50S ribosomal protein bL37



- Molecule 48: Large ribosomal subunit protein uL10

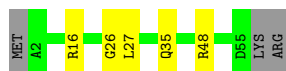


- Molecule 49: Large ribosomal subunit protein uL30

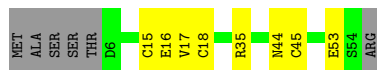


- Molecule 50: Large ribosomal subunit protein bL32

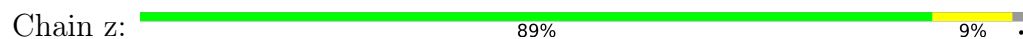




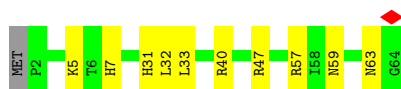
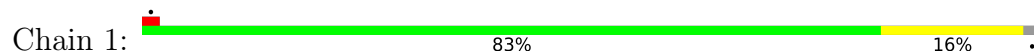
- Molecule 51: Large ribosomal subunit protein bL33A



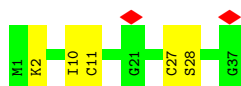
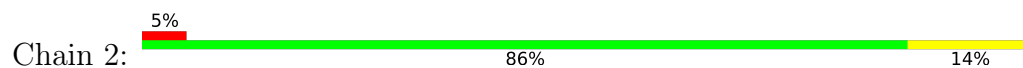
- Molecule 52: Large ribosomal subunit protein bL34



- Molecule 53: Large ribosomal subunit protein bL35



- Molecule 54: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72.704	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	17.694	Depositor
Minimum map value	-13.756	Depositor
Average map value	-0.010	Depositor
Map value standard deviation	0.546	Depositor
Recommended contour level	0.901	Depositor
Map size (Å)	573.696, 573.696, 573.696	wwPDB
Map dimensions	864, 864, 864	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.664, 0.664, 0.664	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.09	0/36308	0.23	2/56653 (0.0%)
2	B	0.19	0/280	0.29	0/359
3	C	0.13	0/1684	0.27	0/2261
4	D	0.13	0/1672	0.31	0/2251
5	E	0.12	0/1312	0.26	0/1772
6	F	0.12	0/782	0.27	0/1059
7	G	0.10	0/1252	0.29	0/1690
8	H	0.12	0/1025	0.24	0/1385
9	I	0.13	0/1012	0.33	0/1362
10	J	0.15	0/802	0.32	0/1086
11	K	0.13	0/873	0.27	0/1180
12	L	0.10	0/969	0.27	0/1294
13	M	0.15	0/942	0.39	0/1260
14	N	0.16	0/488	0.35	0/650
15	O	0.15	0/729	0.31	0/977
16	P	0.13	0/908	0.32	0/1226
17	Q	0.12	0/759	0.30	0/1016
18	R	0.15	0/518	0.34	0/693
19	S	0.11	0/680	0.28	0/915
20	T	0.18	0/663	0.39	0/882
21	V	0.12	0/1822	0.32	0/2457
22	X	0.07	0/128	0.12	0/196
23	Y	0.11	0/71012	0.25	2/110722 (0.0%)
24	U	0.09	0/2821	0.22	0/4396
25	Z	0.17	0/2153	0.41	0/2895
26	a	0.13	0/1609	0.29	0/2165
27	b	0.12	0/1592	0.25	0/2153
28	c	0.14	0/1467	0.31	0/1973
29	d	0.12	0/1369	0.25	0/1848
30	e	0.12	0/986	0.26	0/1303
31	f	0.10	0/1157	0.24	0/1567
32	g	0.12	0/946	0.26	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.13	0/1091	0.32	0/1457
34	i	0.13	0/1118	0.32	0/1506
35	j	0.15	0/945	0.32	0/1267
36	k	0.12	0/966	0.25	0/1298
37	l	0.12	0/921	0.27	0/1236
38	m	0.15	0/1000	0.29	0/1341
39	n	0.13	0/764	0.26	0/1030
40	o	0.15	0/887	0.27	0/1204
41	p	0.15	0/766	0.34	0/1030
42	q	0.09	0/738	0.24	0/987
43	r	0.10	0/1443	0.23	0/1970
44	s	0.14	0/595	0.27	0/798
45	t	0.14	0/478	0.29	0/641
46	u	0.21	0/534	0.38	0/713
47	5	0.15	0/191	0.24	0/247
48	v	0.10	0/925	0.26	0/1246
49	w	0.14	0/477	0.25	0/640
50	x	0.14	0/427	0.25	0/572
51	y	0.16	0/413	0.28	0/553
52	z	0.14	0/380	0.24	0/500
53	1	0.10	0/507	0.22	0/672
54	2	0.10	0/303	0.23	0/401
All	All	0.11	0/156589	0.26	4/234223 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1382	C	OP2-P-O3'	-9.16	80.51	108.00
23	Y	72	G	OP1-P-O3'	-8.73	81.79	108.00
23	Y	72	G	OP2-P-O3'	-8.16	83.52	108.00
1	A	1382	C	OP1-P-O3'	-7.28	86.15	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32439	16316	16319	264	0
2	B	280	343	342	7	0
3	C	1660	1708	1707	20	0
4	D	1641	1669	1668	43	0
5	E	1296	1361	1360	23	0
6	F	771	797	797	11	0
7	G	1232	1282	1282	22	0
8	H	1010	1047	1046	13	0
9	I	994	1050	1050	20	0
10	J	788	820	819	16	0
11	K	855	864	863	15	0
12	L	958	1045	1045	19	0
13	M	935	987	986	30	0
14	N	477	504	499	11	0
15	O	720	761	760	14	0
16	P	891	936	935	14	0
17	Q	748	796	795	16	0
18	R	513	541	537	12	0
19	S	662	677	677	12	0
20	T	660	713	712	29	0
21	V	1793	1839	1839	41	0
22	X	117	63	63	0	0
23	Y	63444	31908	31943	473	0
24	U	2522	1285	1285	16	0
25	Z	2110	2166	2165	36	0
26	a	1587	1631	1630	26	0
27	b	1569	1608	1607	17	0
28	c	1445	1477	1476	28	0
29	d	1348	1400	1399	15	0
30	e	990	1022	1002	10	0
31	f	1130	1167	1167	14	0
32	g	938	1000	1000	9	0
33	h	1078	1152	1151	14	0
34	i	1092	1128	1128	15	0
35	j	928	972	972	12	0
36	k	956	992	991	11	0
37	l	907	938	938	6	0
38	m	988	1039	1038	9	0
39	n	754	803	802	7	0
40	o	873	910	909	6	0
41	p	756	803	802	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	q	732	783	782	11	0
43	r	1428	1444	1443	14	0
44	s	586	602	601	5	0
45	t	470	485	480	4	0
46	u	531	542	541	10	0
47	5	189	206	205	1	0
48	v	918	959	959	9	0
49	w	474	501	500	5	0
50	x	423	464	463	5	0
51	y	405	412	407	4	0
52	z	377	412	411	5	0
53	1	502	541	541	8	0
54	2	299	324	321	3	0
55	1	1	0	0	0	0
55	A	212	0	0	0	0
55	B	1	0	0	0	0
55	F	1	0	0	0	0
55	N	1	0	0	0	0
55	P	1	0	0	0	0
55	R	1	0	0	0	0
55	U	9	0	0	0	0
55	Y	381	0	0	0	0
55	Z	9	0	0	0	0
55	b	1	0	0	0	0
55	c	1	0	0	0	0
55	i	1	0	0	0	0
55	o	1	0	0	0	0
55	p	1	0	0	0	0
55	s	1	0	0	0	0
55	t	1	0	0	0	0
56	2	1	0	0	0	0
56	N	1	0	0	0	0
56	R	1	0	0	0	0
56	t	1	0	0	0	0
56	y	1	0	0	0	0
All	All	144818	97195	97160	1297	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 6.

All (1297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:U:OP2	12:L:94:ARG:NH2	2.03	0.92
23:Y:276:G:N2	23:Y:310:C:O2	2.02	0.92
23:Y:74:C:OP1	46:u:56:ARG:NH1	2.03	0.91
23:Y:981:U:O2'	23:Y:982:A:OP2	1.88	0.91
23:Y:253:C:OP2	53:l:5:LYS:NZ	2.03	0.90
23:Y:316:U:O2'	23:Y:317:G:OP1	1.90	0.89
23:Y:2166:C:OP2	23:Y:2167:U:O2'	1.88	0.89
23:Y:274:C:O2	23:Y:313:G:N2	2.06	0.89
23:Y:621:U:O2'	38:m:49:ASP:OD2	1.91	0.88
1:A:1053:U:OP1	5:E:87:LYS:NZ	2.07	0.88
23:Y:2166:C:O2'	23:Y:2167:U:OP1	1.92	0.87
23:Y:554:A:OP1	52:z:37:ARG:NH1	2.08	0.87
1:A:1058:U:O2'	1:A:1059:G:O5'	1.92	0.87
1:A:149:A:N6	1:A:166:C:O2	2.08	0.86
23:Y:499:G:OP2	23:Y:2630:A:O2'	1.94	0.86
23:Y:1258:C:OP2	31:f:68:LYS:NZ	2.07	0.86
23:Y:324:C:O2	23:Y:452:G:N2	2.07	0.86
1:A:1198:C:OP1	14:N:9:LYS:NZ	2.09	0.85
24:U:10:G:O2'	24:U:11:U:OP1	1.92	0.85
23:Y:361:A:N1	23:Y:441:G:O2'	2.08	0.85
1:A:758:G:O2'	11:K:130:CYS:SG	2.33	0.85
1:A:404:G:OP2	4:D:110:ARG:NH2	2.09	0.85
25:Z:72:LYS:NZ	25:Z:101:GLU:OE1	2.08	0.85
23:Y:2089:C:O2'	23:Y:2090:U:O4'	1.95	0.84
1:A:772:A:O2'	1:A:774:A:N7	2.10	0.84
8:H:5:ASP:OD1	8:H:79:ARG:NH1	2.11	0.83
9:I:146:GLN:NE2	9:I:148:SER:OG	2.11	0.83
23:Y:2727:A:O2'	23:Y:2729:G:OP2	1.96	0.83
1:A:297:G:N2	1:A:300:A:OP2	2.11	0.83
1:A:1261:A:OP1	10:J:9:ARG:NH2	2.11	0.83
23:Y:1493:A:O2'	23:Y:1494:U:OP2	1.97	0.83
23:Y:1252:G:O6	47:5:6:ARG:NH2	2.11	0.83
1:A:209:A:OP1	20:T:60:LYS:NZ	2.11	0.83
23:Y:329:U:O2	23:Y:446:G:O6	1.95	0.83
23:Y:1634:C:O2'	23:Y:1635:A:OP1	1.95	0.82
1:A:124:G:O2'	17:Q:20:ARG:NH1	2.12	0.82
23:Y:1010:U:O2'	23:Y:1011:A:OP1	1.97	0.82
23:Y:1007:G:N2	23:Y:1008:G:N7	2.27	0.82
23:Y:2088:C:O2'	23:Y:2089:C:O5'	1.97	0.82
1:A:592:U:O3'	4:D:76:ARG:NH2	2.13	0.81
1:A:157:A:N6	1:A:343:U:O2'	2.13	0.81
1:A:1386:C:O2	1:A:1483:A:N6	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:33:ARG:NH1	20:T:37:GLU:OE1	2.13	0.81
23:Y:993:G:N2	23:Y:1015:A:OP2	2.15	0.80
1:A:998:G:O2'	1:A:999:A:O4'	1.98	0.80
23:Y:361:A:O2'	23:Y:362:A:O4'	1.98	0.80
1:A:1482:U:O2'	1:A:1483:A:OP2	1.98	0.80
23:Y:1379:G:OP1	50:x:16:ARG:NH2	2.14	0.80
9:I:62:LYS:O	9:I:66:GLN:NE2	2.15	0.80
23:Y:1532:G:O2'	23:Y:1533:U:O4'	2.00	0.80
23:Y:1730:U:O2'	23:Y:1731:A:OP2	2.01	0.79
23:Y:199:U:O2	23:Y:474:G:N2	2.16	0.78
23:Y:2087:C:N4	23:Y:2095:G:O6	2.14	0.78
35:j:57:LYS:O	35:j:62:ASN:ND2	2.15	0.78
1:A:1434:U:O2'	1:A:1435:U:O4'	2.01	0.78
1:A:1484:A:O2'	2:B:8:ARG:NH2	2.16	0.78
1:A:1080:C:OP2	21:V:95:ARG:NH1	2.16	0.78
9:I:27:GLN:OE1	9:I:38:ARG:NH2	2.16	0.78
23:Y:79:G:O2'	23:Y:80:G:O4'	2.01	0.78
23:Y:2796:A:OP2	26:a:156:THR:OG1	2.00	0.78
23:Y:747:A:N6	23:Y:768:G:O2'	2.17	0.78
23:Y:2914:A:OP1	35:j:9:ARG:NH2	2.16	0.77
23:Y:1530:G:N2	23:Y:1805:G:O6	2.17	0.77
1:A:1184:C:OP1	14:N:2:ALA:N	2.18	0.77
1:A:1432:C:N3	1:A:1433:C:N4	2.31	0.77
1:A:544:C:OP2	12:L:12:ARG:NH1	2.16	0.77
51:y:44:ASN:OD1	51:y:45:CYS:N	2.18	0.77
23:Y:2151:A:O2'	23:Y:2152:A:O4'	2.01	0.77
23:Y:1186:G:N2	23:Y:1213:A:O2'	2.18	0.77
23:Y:1260:C:O2'	31:f:27:ARG:NH2	2.18	0.77
23:Y:2580:G:OP1	44:s:24:LYS:NZ	2.18	0.76
25:Z:133:LEU:O	25:Z:168:LYS:NZ	2.17	0.76
1:A:1027:G:O2'	1:A:1196:G:O2'	2.03	0.76
1:A:100:G:OP1	20:T:16:ARG:NH2	2.18	0.76
1:A:423:G:N2	1:A:423:G:OP2	2.19	0.76
1:A:996:G:OP1	19:S:18:LYS:NZ	2.19	0.76
23:Y:313:G:O2'	23:Y:314:G:O4'	2.02	0.76
9:I:126:ARG:NH1	9:I:127:ASP:O	2.18	0.76
1:A:1221:U:O4	7:G:109:ARG:NH2	2.19	0.76
23:Y:2559:A:OP2	36:k:24:ARG:NH1	2.19	0.76
23:Y:3020:U:O2'	23:Y:3021:A:O5'	2.02	0.76
1:A:1504:G:N7	2:B:15:LYS:NZ	2.34	0.75
4:D:52:GLU:OE2	4:D:55:LYS:NZ	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1506:U:OP1	11:K:137:ARG:NH2	2.19	0.75
8:H:79:ARG:NE	8:H:81:SER:O	2.20	0.75
23:Y:81:A:OP1	42:q:4:HIS:NE2	2.19	0.75
23:Y:3086:U:OP2	23:Y:3087:G:O2'	2.03	0.75
1:A:676:A:N3	1:A:766:G:O2'	2.19	0.74
20:T:47:ALA:O	20:T:51:LEU:HD12	1.87	0.74
23:Y:2482:U:O2'	23:Y:2651:C:OP2	2.05	0.74
1:A:210:A:HO2'	1:A:221:G:HO2'	1.21	0.74
1:A:1498:C:OP2	2:B:22:ARG:NH2	2.19	0.74
23:Y:473:C:O2'	23:Y:476:G:N2	2.20	0.74
23:Y:2580:G:O2'	23:Y:2581:G:O5'	2.04	0.74
23:Y:1996:U:OP2	23:Y:2001:A:N6	2.15	0.74
1:A:1232:A:N6	1:A:1268:C:O2	2.21	0.74
23:Y:1440:C:N3	40:o:93:ARG:NH2	2.36	0.74
28:c:141:GLU:OE2	28:c:143:SER:OG	2.02	0.73
33:h:94:GLY:N	33:h:97:GLU:OE2	2.21	0.73
37:l:49:ARG:NE	37:l:56:GLU:OE2	2.21	0.73
1:A:23:C:OP1	5:E:160:ASN:ND2	2.22	0.73
17:Q:83:SER:O	17:Q:87:ARG:NH1	2.22	0.73
23:Y:2235:C:OP2	40:o:23:LYS:NZ	2.14	0.73
1:A:823:U:O4	1:A:826:U:N3	2.22	0.72
1:A:1159:G:OP1	9:I:115:ARG:NH1	2.23	0.72
49:w:21:GLU:OE1	49:w:24:ARG:NH1	2.23	0.72
1:A:193:C:O2	1:A:194:A:N6	2.22	0.72
23:Y:452:G:O2'	23:Y:453:U:O4'	2.04	0.72
23:Y:1185:A:O2'	23:Y:1186:G:O4'	2.06	0.72
23:Y:1851:G:N7	23:Y:1853:A:N6	2.37	0.72
1:A:210:A:O2'	1:A:221:G:O2'	1.95	0.72
13:M:4:LEU:HD21	13:M:53:VAL:CG1	2.19	0.72
20:T:46:LYS:O	20:T:50:LEU:HD23	1.89	0.72
23:Y:684:G:O2'	23:Y:685:G:OP1	2.08	0.72
1:A:954:C:O5'	10:J:59:LYS:NZ	2.22	0.72
23:Y:419:G:O6	23:Y:420:G:N2	2.23	0.72
43:r:122:THR:HG23	43:r:181:VAL:HG13	1.71	0.72
1:A:485:G:O2'	1:A:486:G:OP1	2.07	0.72
23:Y:1224:G:O2'	48:v:28:TYR:OH	2.08	0.72
21:V:156:LYS:O	21:V:157:VAL:HG22	1.90	0.71
23:Y:980:C:O2'	23:Y:981:U:O5'	2.07	0.71
29:d:166:GLU:N	29:d:166:GLU:OE2	2.23	0.71
33:h:123:ASP:OD1	33:h:143:SER:OG	2.08	0.71
43:r:6:ASN:OD1	43:r:7:ILE:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:U:O2	1:A:1500:G:O2'	2.05	0.71
8:H:48:ASP:OD2	8:H:49:TYR:N	2.22	0.71
23:Y:2616:A:C2	33:h:55:MET:HE1	2.24	0.71
23:Y:452:G:O2'	23:Y:453:U:O5'	2.08	0.71
23:Y:1482:A:O3'	52:z:28:ARG:NH2	2.22	0.71
1:A:11:G:O6	5:E:122:ARG:NH2	2.24	0.71
23:Y:1532:G:O2'	23:Y:1533:U:O5'	2.09	0.71
23:Y:2537:C:O4'	28:c:44:ASN:ND2	2.23	0.71
21:V:4:VAL:HG13	21:V:8:GLN:OE1	1.91	0.71
23:Y:2062:G:OP2	25:Z:256:ARG:NH2	2.24	0.71
10:J:23:ARG:NH2	10:J:27:GLU:OE2	2.24	0.70
23:Y:2558:C:N3	44:s:75:ARG:NH2	2.39	0.70
1:A:260:G:OP1	20:T:75:LYS:NZ	2.23	0.70
1:A:376:G:O3'	16:P:6:LYS:NZ	2.25	0.70
23:Y:276:G:N1	23:Y:310:C:N3	2.39	0.70
23:Y:313:G:O2'	23:Y:314:G:O5'	2.09	0.70
23:Y:725:A:OP2	53:1:47:ARG:NH2	2.24	0.70
23:Y:1203:A:O2'	23:Y:1204:A:O4'	2.10	0.70
1:A:324:G:OP1	20:T:17:ARG:NH2	2.24	0.70
1:A:975:G:O2'	1:A:976:A:N7	2.25	0.70
23:Y:336:C:O2'	23:Y:337:U:OP1	2.08	0.70
42:q:86:ARG:NH2	42:q:104:ASP:OD2	2.25	0.70
28:c:45:MET:HE1	28:c:64:LEU:HD21	1.74	0.70
23:Y:2043:C:O2'	23:Y:2195:U:OP2	2.10	0.69
1:A:606:U:OP1	16:P:19:ARG:NH1	2.24	0.69
42:q:13:SER:OG	42:q:70:ASN:OD1	2.11	0.69
7:G:59:VAL:HG22	7:G:63:LYS:HE2	1.72	0.69
23:Y:287:A:N6	23:Y:299:G:O2'	2.24	0.69
1:A:156:G:O2'	1:A:158:A:N7	2.25	0.69
23:Y:1204:A:O2'	23:Y:1205:G:N7	2.26	0.69
23:Y:1426:G:N2	23:Y:1426:G:OP2	2.26	0.69
20:T:81:LEU:HD12	20:T:85:LYS:HZ1	1.57	0.69
1:A:1203:G:OP2	1:A:1304:C:N4	2.24	0.69
13:M:4:LEU:HD11	13:M:53:VAL:HG13	1.74	0.69
25:Z:66:ASP:OD2	25:Z:103:ARG:NH1	2.26	0.69
1:A:487:C:OP2	1:A:488:C:O2'	2.02	0.69
1:A:1351:G:OP2	9:I:134:LYS:NZ	2.25	0.69
1:A:810:G:O2'	21:V:21:ARG:NH1	2.24	0.68
23:Y:1076:A:O2'	23:Y:1077:A:O4'	2.09	0.68
13:M:104:LYS:HE3	13:M:104:LYS:HA	1.74	0.68
30:e:26:VAL:O	30:e:30:LEU:HD23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1260:A:O2'	1:A:1263:C:N4	2.25	0.68
1:A:1279:U:OP1	13:M:44:ARG:NH2	2.27	0.68
53:1:59:ASN:OD1	53:1:63:ASN:ND2	2.27	0.68
15:O:74:ASP:OD1	15:O:75:VAL:N	2.27	0.68
1:A:194:A:O2'	1:A:195:U:O4'	2.10	0.67
1:A:714:G:O3'	18:R:69:LYS:NZ	2.27	0.67
20:T:4:ILE:O	20:T:8:ILE:HD12	1.93	0.67
21:V:142:ASN:OD1	21:V:143:LYS:N	2.27	0.67
23:Y:679:G:OP2	33:h:24:ARG:NH2	2.26	0.67
1:A:552:A:HO2'	1:A:898:G:HO2'	1.37	0.67
4:D:142:GLU:O	4:D:146:ASN:ND2	2.27	0.67
23:Y:2580:G:O2'	23:Y:2581:G:O4'	2.09	0.67
23:Y:1198:C:O3'	30:e:128:LYS:NZ	2.27	0.67
33:h:115:ASP:OD1	33:h:116:GLY:N	2.28	0.67
4:D:169:VAL:HG21	4:D:174:ARG:HH21	1.58	0.67
1:A:92:A:O2'	1:A:93:C:O5'	2.12	0.67
21:V:154:MET:O	21:V:156:LYS:N	2.27	0.66
41:p:34:HIS:ND1	41:p:36:ASP:OD1	2.27	0.66
23:Y:639:C:O2'	23:Y:640:G:O5'	2.13	0.66
25:Z:126:LYS:O	25:Z:129:ASN:ND2	2.28	0.66
1:A:142:U:O2	1:A:174:G:O6	2.13	0.66
1:A:1249:G:N2	1:A:1309:C:O4'	2.28	0.66
3:C:56:ILE:HG22	3:C:65:VAL:HG12	1.76	0.66
23:Y:1201:G:N2	23:Y:1204:A:OP2	2.28	0.66
23:Y:788:C:OP1	23:Y:916:G:N2	2.28	0.66
1:A:1291:G:N2	1:A:1310:C:O2	2.20	0.66
1:A:958:G:O2'	1:A:959:A:OP2	2.13	0.66
23:Y:566:A:N7	23:Y:568:A:N6	2.44	0.66
23:Y:1847:U:O4	23:Y:1848:A:N6	2.27	0.66
23:Y:1930:C:OP2	23:Y:1931:A:O2'	2.08	0.66
48:v:45:ASP:OD1	48:v:46:SER:N	2.28	0.66
1:A:1251:G:HO2'	1:A:1295:U:HO2'	1.37	0.66
21:V:210:ALA:O	21:V:214:THR:HG23	1.95	0.66
23:Y:1683:C:HO2'	23:Y:2926:A:HO2'	1.43	0.65
23:Y:1092:G:O2'	23:Y:1093:A:OP2	2.13	0.65
49:w:8:GLN:HB2	49:w:28:LEU:HD23	1.77	0.65
23:Y:662:G:O4'	23:Y:1101:A:N6	2.30	0.65
23:Y:1441:C:HO2'	23:Y:2234:G:HO2'	1.40	0.65
30:e:87:VAL:O	30:e:89:LYS:N	2.29	0.65
1:A:953:G:O2'	1:A:1348:G:O2'	2.14	0.65
21:V:4:VAL:HG21	21:V:212:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:1541:G:N2	23:Y:1631:A:N1	2.42	0.65
23:Y:2579:C:N4	23:Y:2580:G:H22	1.95	0.65
25:Z:146:GLU:OE2	25:Z:152:GLY:N	2.30	0.65
43:r:28:ARG:NH1	43:r:93:GLN:O	2.30	0.65
30:e:67:SER:HG	30:e:68:PHE:N	1.94	0.65
1:A:194:A:O2'	1:A:195:U:O5'	2.14	0.64
35:j:37:THR:HG22	35:j:39:PRO:HD2	1.79	0.64
28:c:45:MET:CE	28:c:64:LEU:HD21	2.28	0.64
23:Y:363:A:N1	23:Y:439:C:O2'	2.27	0.64
1:A:745:G:H1	1:A:792:G:HO2'	1.44	0.64
23:Y:470:G:N2	23:Y:481:C:N3	2.45	0.64
1:A:187:U:O2	1:A:201:G:O6	2.16	0.63
1:A:1057:G:O2'	1:A:1059:G:O6	2.16	0.63
34:i:84:GLY:O	34:i:85:SER:OG	2.14	0.63
34:i:114:ALA:O	34:i:118:LEU:HD23	1.99	0.63
23:Y:1720:G:N2	25:Z:99:ASP:O	2.31	0.63
21:V:162:TRP:HH2	21:V:214:THR:HG22	1.64	0.63
23:Y:2578:A:O2'	44:s:35:GLU:OE2	2.10	0.63
36:k:83:ARG:O	36:k:87:LEU:HD23	1.99	0.63
38:m:89:GLU:OE1	39:n:8:LYS:NZ	2.27	0.63
20:T:81:LEU:HD12	20:T:85:LYS:NZ	2.13	0.63
23:Y:392:A:O2'	23:Y:393:U:OP2	2.14	0.63
23:Y:2087:C:N3	23:Y:2095:G:N1	2.45	0.63
1:A:1109:C:O2'	1:A:1110:A:O5'	2.14	0.63
1:A:1231:A:N3	1:A:1353:G:O2'	2.32	0.63
23:Y:218:A:N3	23:Y:234:U:O2'	2.32	0.63
13:M:5:VAL:HG12	13:M:5:VAL:O	1.98	0.63
15:O:8:LYS:O	15:O:12:LEU:HD23	1.98	0.63
23:Y:274:C:N4	23:Y:275:C:H41	1.96	0.63
42:q:11:VAL:HA	42:q:71:VAL:HG12	1.80	0.63
1:A:1106:U:OP1	10:J:7:ARG:NH2	2.32	0.63
5:E:140:LEU:HD13	5:E:148:ILE:HG21	1.80	0.63
20:T:51:LEU:HD13	20:T:83:LEU:HD12	1.80	0.63
1:A:173:C:OP1	20:T:64:LYS:NZ	2.24	0.62
7:G:31:LEU:HD21	7:G:36:LYS:HA	1.80	0.62
25:Z:125:ILE:HG22	25:Z:125:ILE:O	1.99	0.62
1:A:25:G:H21	1:A:896:A:H62	1.47	0.62
1:A:323:U:O3'	20:T:17:ARG:NH1	2.32	0.62
23:Y:1533:U:O2	23:Y:1803:A:O2'	2.15	0.62
21:V:18:HIS:NE2	21:V:205:ASP:OD2	2.33	0.62
23:Y:1843:C:N4	23:Y:1844:A:N1	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:69:ASP:O	13:M:73:GLU:OE1	2.17	0.62
1:A:1289:U:O4	1:A:1313:G:N2	2.32	0.62
1:A:1149:C:O2'	1:A:1150:A:OP2	2.06	0.62
1:A:1303:U:O2'	19:S:78:ARG:NH2	2.33	0.62
8:H:115:ASP:OD1	8:H:116:ARG:N	2.32	0.62
11:K:130:CYS:SG	11:K:131:ARG:N	2.73	0.62
12:L:107:VAL:HG13	12:L:110:ARG:HB2	1.81	0.62
23:Y:2586:G:OP1	53:1:40:ARG:NH2	2.32	0.62
28:c:67:ILE:HG23	28:c:68:THR:HG23	1.82	0.61
1:A:192:G:O3'	17:Q:17:ARG:NH2	2.33	0.61
1:A:858:A:H1'	8:H:12:THR:HG21	1.83	0.61
23:Y:277:U:O4	23:Y:309:G:O6	2.18	0.61
23:Y:1063:G:O6	23:Y:1090:G:N2	2.33	0.61
23:Y:288:U:N3	23:Y:299:G:O6	2.32	0.61
1:A:50:G:O2'	1:A:365:U:O2'	2.07	0.61
29:d:88:MET:HE1	29:d:146:SER:OG	2.00	0.61
23:Y:1073:G:O2'	23:Y:1076:A:N6	2.34	0.61
23:Y:2178:G:O2'	23:Y:2180:U:O4	2.13	0.61
28:c:62:ASN:O	28:c:66:LEU:HD23	2.00	0.61
26:a:114:VAL:HG22	26:a:208:VAL:HG12	1.82	0.61
6:F:82:ASN:OD1	6:F:83:GLU:N	2.33	0.61
21:V:100:MET:HG2	21:V:101:LEU:HD12	1.83	0.61
30:e:107:VAL:HG13	30:e:130:ILE:HD11	1.82	0.60
4:D:156:THR:O	4:D:156:THR:HG22	1.99	0.60
21:V:51:ASP:O	21:V:55:GLU:OE1	2.18	0.60
23:Y:2054:C:N4	23:Y:2123:A:N7	2.49	0.60
1:A:1129:U:O3'	9:I:31:ARG:NH2	2.34	0.60
20:T:48:SER:O	20:T:52:HIS:ND1	2.34	0.60
23:Y:274:C:O2'	23:Y:323:C:OP1	2.19	0.60
19:S:63:THR:HG23	19:S:65:ALA:H	1.67	0.60
1:A:1297:U:O2'	1:A:1342:A:N3	2.27	0.60
1:A:1300:A:O2'	19:S:37:ARG:NH1	2.33	0.60
23:Y:1631:A:N6	23:Y:1632:G:O6	2.34	0.60
23:Y:2708:G:OP1	34:i:45:ARG:NH1	2.35	0.60
45:t:13:GLY:N	45:t:29:TRP:O	2.35	0.60
1:A:810:G:O2'	21:V:21:ARG:NH2	2.35	0.60
23:Y:555:G:N7	52:z:42:ARG:NH2	2.50	0.60
10:J:14:ASP:OD1	10:J:17:ALA:HB3	2.02	0.60
23:Y:1189:G:N2	23:Y:1207:G:N3	2.50	0.60
23:Y:1927:C:O2'	23:Y:3080:A:N3	2.34	0.60
13:M:19:LEU:HD12	13:M:22:ILE:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:336:C:HO2'	23:Y:337:U:P	2.24	0.60
23:Y:2724:U:O2'	23:Y:2728:U:OP1	2.20	0.59
25:Z:71:ASP:OD2	25:Z:72:LYS:N	2.35	0.59
31:f:14:SER:N	31:f:52:ASP:OD2	2.35	0.59
1:A:1251:G:O2'	1:A:1295:U:O2'	2.14	0.59
26:a:160:VAL:HG12	26:a:160:VAL:O	2.01	0.59
1:A:777:C:OP1	11:K:136:ARG:NH1	2.35	0.59
17:Q:63:ASP:OD1	17:Q:64:GLU:N	2.35	0.59
23:Y:1259:U:OP2	31:f:65:SER:OG	2.19	0.59
48:v:35:ASN:OD1	48:v:36:LEU:N	2.35	0.59
23:Y:1849:G:H21	23:Y:1853:A:H62	1.48	0.59
23:Y:1349:U:O2'	23:Y:1350:G:O5'	2.21	0.59
12:L:21:THR:HG23	12:L:95:TYR:CE1	2.38	0.59
13:M:2:ALA:O	13:M:9:LEU:N	2.35	0.59
23:Y:2022:U:OP1	25:Z:252:LYS:NZ	2.29	0.59
1:A:960:A:N6	1:A:1300:A:N7	2.50	0.58
23:Y:551:G:N2	23:Y:554:A:OP2	2.36	0.58
23:Y:2236:G:O2'	23:Y:2237:A:O5'	2.17	0.58
26:a:63:ILE:HG22	26:a:65:PRO:HD2	1.84	0.58
1:A:133:C:O2'	16:P:65:GLN:NE2	2.35	0.58
1:A:771:G:O6	1:A:772:A:N6	2.36	0.58
13:M:86:CYS:SG	13:M:87:TYR:N	2.76	0.58
23:Y:322:A:O2'	23:Y:323:C:OP1	2.18	0.58
23:Y:1482:A:O2'	52:z:28:ARG:NH2	2.37	0.58
23:Y:1702:A:N1	23:Y:1731:A:N6	2.52	0.58
1:A:746:A:N7	1:A:793:U:O4	2.35	0.58
10:J:42:LEU:HD11	10:J:73:LEU:HG	1.86	0.58
1:A:1148:U:OP1	1:A:1150:A:N6	2.34	0.58
11:K:122:VAL:HG23	11:K:122:VAL:O	2.02	0.58
23:Y:159:A:OP2	23:Y:164:A:N6	2.33	0.58
23:Y:1075:U:O4	34:i:17:GLN:NE2	2.37	0.58
1:A:1249:G:N3	1:A:1308:C:O2'	2.36	0.58
1:A:426:U:OP1	4:D:29:ARG:NH1	2.37	0.58
1:A:553:A:O2'	1:A:554:A:O4'	2.22	0.58
27:b:49:THR:HG23	27:b:49:THR:O	2.03	0.58
28:c:170:ASP:OD1	28:c:171:ALA:N	2.37	0.58
1:A:1205:U:O2'	1:A:1206:U:OP1	2.18	0.58
11:K:70:PHE:CZ	11:K:74:LEU:HD21	2.38	0.58
23:Y:176:G:OP2	23:Y:176:G:N2	2.30	0.58
30:e:110:ILE:HA	30:e:113:THR:HG22	1.86	0.58
19:S:12:ASP:OD2	19:S:35:SER:OG	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:111:LEU:HD22	21:V:151:ILE:HG22	1.86	0.57
46:u:41:LEU:HD21	46:u:46:ARG:HD2	1.85	0.57
23:Y:959:U:O2'	23:Y:960:G:OP1	2.21	0.57
23:Y:3043:G:O2'	23:Y:3045:C:OP2	2.12	0.57
28:c:29:TYR:OH	28:c:172:GLU:OE2	2.21	0.57
23:Y:251:A:OP1	53:1:7:HIS:NE2	2.35	0.57
1:A:1504:G:OP2	2:B:11:ARG:NH2	2.35	0.57
5:E:40:VAL:HG12	5:E:62:VAL:HG12	1.85	0.57
23:Y:274:C:C2	23:Y:313:G:N2	2.72	0.57
37:l:34:GLY:O	37:l:35:SER:OG	2.18	0.57
40:o:32:ARG:NH1	40:o:81:VAL:O	2.38	0.57
23:Y:1381:G:N2	23:Y:2237:A:OP2	2.38	0.57
23:Y:2299:C:OP2	23:Y:2462:G:N2	2.38	0.57
23:Y:638:U:O2'	23:Y:639:C:OP2	2.20	0.57
25:Z:181:GLU:N	25:Z:181:GLU:OE1	2.38	0.57
50:x:26:GLY:C	50:x:27:LEU:HD22	2.28	0.57
1:A:363:A:O2'	1:A:364:A:O4'	2.20	0.57
23:Y:2699:C:O2'	23:Y:2701:U:OP1	2.20	0.57
1:A:1063:U:O2'	1:A:1082:A:OP2	2.22	0.57
4:D:140:VAL:HG11	4:D:150:PHE:CZ	2.40	0.57
1:A:986:G:N2	1:A:987:A:N3	2.49	0.57
20:T:18:ARG:NH1	20:T:22:GLN:OE1	2.38	0.57
23:Y:2154:G:O2'	23:Y:2155:U:OP2	2.22	0.57
23:Y:2802:G:N7	26:a:150:SER:OG	2.36	0.57
8:H:26:THR:C	8:H:27:LEU:HD12	2.30	0.56
20:T:15:GLU:O	20:T:19:LEU:HD23	2.05	0.56
21:V:6:MET:HE3	21:V:43:LEU:HD12	1.86	0.56
21:V:148:LEU:CD1	21:V:151:ILE:HD12	2.35	0.56
24:U:10:G:HO2'	24:U:11:U:P	2.25	0.56
49:w:39:ASP:OD1	49:w:39:ASP:O	2.23	0.56
1:A:1109:C:HO2'	1:A:1110:A:P	2.28	0.56
29:d:158:TYR:O	29:d:172:ARG:NH2	2.37	0.56
1:A:1011:U:O2'	1:A:1012:U:O5'	2.20	0.56
1:A:1104:G:HO2'	1:A:1126:G:H1	1.51	0.56
1:A:1302:C:N3	19:S:36:ARG:NH1	2.53	0.56
7:G:24:THR:O	7:G:28:ASN:ND2	2.38	0.56
13:M:69:ASP:OD1	13:M:70:LEU:N	2.39	0.56
17:Q:42:ASP:OD1	17:Q:43:ARG:N	2.38	0.56
23:Y:2503:G:N7	44:s:14:ARG:NH1	2.53	0.56
10:J:56:HIS:O	10:J:57:LYS:HG2	2.05	0.56
20:T:24:VAL:O	20:T:27:SER:OG	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:A:OP1	5:E:77:LYS:NZ	2.33	0.56
23:Y:1377:A:C2	23:Y:1378:U:C5	2.94	0.56
1:A:408:G:O2'	4:D:104:ARG:NH1	2.38	0.55
4:D:133:SER:N	4:D:136:ASP:OD2	2.39	0.55
17:Q:37:VAL:HG12	17:Q:60:LYS:HG2	1.87	0.55
23:Y:2406:U:O4	23:Y:2410:A:O2'	2.23	0.55
23:Y:2008:A:N6	23:Y:2045:G:O2'	2.38	0.55
25:Z:220:THR:O	25:Z:221:VAL:HG22	2.06	0.55
43:r:119:THR:OG1	43:r:122:THR:OG1	2.23	0.55
1:A:1305:G:N2	1:A:1343:G:O2'	2.40	0.55
5:E:187:GLU:N	5:E:187:GLU:OE2	2.39	0.55
16:P:69:PRO:O	16:P:73:LEU:HD23	2.06	0.55
23:Y:1046:C:O2'	23:Y:1047:A:OP2	2.22	0.55
23:Y:1899:G:O2'	23:Y:1979:A:N3	2.27	0.55
23:Y:897:A:C6	25:Z:226:MET:HE1	2.42	0.55
21:V:148:LEU:HD11	21:V:151:ILE:HB	1.88	0.55
23:Y:1128:A:OP1	38:m:66:ASN:ND2	2.36	0.55
26:a:9:THR:HG23	26:a:204:GLY:O	2.07	0.55
23:Y:2044:U:OP2	25:Z:222:ARG:NH2	2.39	0.55
23:Y:844:G:O5'	25:Z:208:LYS:NZ	2.39	0.55
23:Y:1785:C:O2'	23:Y:1787:A:N7	2.38	0.55
1:A:660:C:O2'	25:Z:166:LEU:HD23	2.06	0.55
41:p:91:LYS:HE2	41:p:91:LYS:HA	1.89	0.55
1:A:1249:G:O2'	1:A:1250:A:O5'	2.25	0.55
7:G:12:LEU:HD21	7:G:24:THR:OG1	2.07	0.55
23:Y:1201:G:O2'	23:Y:1203:A:N7	2.35	0.55
26:a:135:GLN:OE1	26:a:144:VAL:HG12	2.06	0.55
1:A:450:G:OP2	1:A:451:A:O2'	2.25	0.55
16:P:86:LEU:HB2	16:P:87:PRO:HD3	1.89	0.55
23:Y:2124:A:O2'	23:Y:2125:A:OP1	2.23	0.55
23:Y:89:A:O2'	23:Y:90:C:OP1	2.23	0.54
1:A:1380:C:OP2	5:E:54:ARG:NH2	2.40	0.54
13:M:71:ARG:O	13:M:75:GLN:OE1	2.24	0.54
23:Y:2323:G:O2'	23:Y:2405:A:OP2	2.23	0.54
13:M:81:LYS:HD3	13:M:84:ILE:HD11	1.88	0.54
23:Y:565:A:O2'	23:Y:566:A:O5'	2.25	0.54
23:Y:726:A:O3'	33:h:69:ASN:ND2	2.39	0.54
23:Y:1938:G:N2	23:Y:1939:U:O4	2.40	0.54
1:A:1231:A:N6	1:A:1268:C:O2	2.40	0.54
14:N:22:THR:OG1	14:N:33:VAL:HG11	2.07	0.54
23:Y:980:C:HO2'	23:Y:981:U:P	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:899:G:O6	25:Z:229:VAL:HG21	2.07	0.54
23:Y:958:A:N6	23:Y:1053:G:O6	2.40	0.54
51:y:15:CYS:SG	51:y:16:GLU:N	2.79	0.54
26:a:144:VAL:HG12	26:a:144:VAL:O	2.08	0.54
29:d:90:ILE:HD12	29:d:163:VAL:HG12	1.90	0.54
51:y:35:ARG:NH2	51:y:53:GLU:O	2.41	0.54
17:Q:32:MET:HE3	17:Q:35:THR:HG22	1.90	0.54
1:A:1391:A:O2'	23:Y:2136:A:N3	2.35	0.54
23:Y:1022:C:OP1	34:i:24:GLY:N	2.33	0.54
23:Y:1033:A:O2'	23:Y:1034:U:O5'	2.23	0.54
33:h:51:GLU:OE2	53:l:57:ARG:NH2	2.38	0.54
1:A:779:G:O6	1:A:780:G:N2	2.41	0.54
23:Y:1165:G:O2'	23:Y:1228:A:N6	2.32	0.54
23:Y:3107:G:O2'	23:Y:3108:G:OP2	2.18	0.54
3:C:59:THR:HG23	3:C:59:THR:O	2.07	0.53
18:R:74:VAL:HG13	18:R:76:LEU:HD13	1.90	0.53
23:Y:2537:C:OP1	28:c:75:ARG:NE	2.41	0.53
42:q:75:ASP:OD1	42:q:76:SER:N	2.41	0.53
1:A:485:G:O2'	1:A:486:G:P	2.66	0.53
17:Q:41:GLU:OE2	17:Q:43:ARG:NH2	2.41	0.53
23:Y:723:C:N4	23:Y:724:G:O6	2.41	0.53
23:Y:1096:G:O6	23:Y:1097:A:N6	2.41	0.53
46:u:15:ASP:OD1	46:u:16:ASP:N	2.42	0.53
4:D:152:ILE:HD12	4:D:152:ILE:H	1.73	0.53
5:E:182:ARG:NH2	5:E:189:VAL:HG12	2.23	0.53
23:Y:2870:C:OP2	23:Y:2956:G:O2'	2.24	0.53
24:U:60:G:H4'	36:k:12:GLU:OE2	2.08	0.53
1:A:669:C:N4	1:A:670:G:O6	2.42	0.53
4:D:175:ILE:O	4:D:176:LEU:HD22	2.08	0.53
1:A:933:G:O2'	1:A:952:C:O2'	2.22	0.53
1:A:1300:A:OP1	19:S:3:ARG:NH2	2.42	0.53
5:E:179:ALA:HB2	5:E:189:VAL:HG21	1.90	0.53
23:Y:1092:G:HO2'	23:Y:1093:A:P	2.31	0.53
4:D:135:TYR:O	16:P:102:LYS:NZ	2.41	0.53
6:F:28:ASN:OD1	6:F:29:VAL:N	2.41	0.53
48:v:82:VAL:HG23	48:v:82:VAL:O	2.08	0.53
8:H:76:GLY:C	8:H:77:LEU:HD12	2.33	0.53
11:K:130:CYS:HG	11:K:131:ARG:H	1.56	0.53
12:L:63:VAL:HG21	12:L:95:TYR:CE2	2.44	0.53
23:Y:905:U:H2'	23:Y:905:U:O2	2.09	0.53
23:Y:1133:G:O6	23:Y:1267:A:N6	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:2050:C:O2'	23:Y:2193:A:N1	2.41	0.53
23:Y:2085:C:O2'	23:Y:2086:U:O5'	2.27	0.53
1:A:1244:G:O6	1:A:1254:G:N2	2.42	0.53
23:Y:1004:C:O2'	23:Y:1005:A:OP1	2.20	0.53
29:d:59:GLU:OE2	29:d:61:ARG:N	2.40	0.53
23:Y:974:G:N2	23:Y:1032:A:OP2	2.42	0.52
23:Y:2973:A:OP2	23:Y:2974:A:O2'	2.22	0.52
10:J:23:ARG:O	10:J:27:GLU:OE1	2.26	0.52
23:Y:3009:U:OP1	26:a:44:ARG:NH2	2.42	0.52
34:i:1:MET:HE3	34:i:1:MET:HA	1.92	0.52
23:Y:160:A:OP2	23:Y:161:U:O2'	2.23	0.52
29:d:149:ILE:O	29:d:152:LEU:HD13	2.10	0.52
1:A:1242:A:OP2	1:A:1255:G:N2	2.42	0.52
23:Y:1099:A:OP2	23:Y:1100:C:N4	2.42	0.52
46:u:48:ARG:O	46:u:52:GLN:OE1	2.27	0.52
1:A:22:C:OP1	5:E:157:ASN:ND2	2.43	0.52
1:A:463:C:OP2	1:A:464:G:O2'	2.24	0.52
1:A:958:G:OP2	1:A:1340:U:O2'	2.27	0.52
16:P:104:ASP:OD1	16:P:105:LEU:N	2.43	0.52
23:Y:1000:C:H2'	23:Y:1001:C:C1'	2.40	0.52
23:Y:1349:U:C2'	23:Y:1350:G:O5'	2.57	0.52
29:d:90:ILE:CD1	29:d:163:VAL:HG12	2.40	0.52
1:A:209:A:N3	1:A:222:U:O2'	2.41	0.52
1:A:1183:U:H1'	14:N:42:ILE:HD11	1.91	0.52
6:F:30:ILE:CD1	6:F:75:LEU:HD22	2.40	0.52
23:Y:22:U:C2'	23:Y:23:G:O5'	2.58	0.52
18:R:37:LEU:O	18:R:40:THR:HG22	2.09	0.52
20:T:85:LYS:HD3	20:T:85:LYS:N	2.25	0.52
21:V:51:ASP:O	21:V:54:TYR:HB3	2.09	0.52
21:V:188:ASP:OD1	21:V:189:THR:N	2.40	0.52
23:Y:2070:A:N7	23:Y:2113:A:N6	2.58	0.52
43:r:54:PHE:O	43:r:58:LEU:HD23	2.09	0.52
8:H:13:ARG:HD2	8:H:27:LEU:HD11	1.92	0.52
23:Y:2698:C:O2	23:Y:2698:C:H2'	2.09	0.52
27:b:103:PRO:HD2	27:b:106:MET:HE3	1.91	0.52
1:A:745:G:N1	1:A:792:G:O2'	2.41	0.52
23:Y:78:G:C6	23:Y:79:G:N2	2.78	0.52
23:Y:1888:C:H2'	23:Y:1889:U:O4'	2.10	0.52
23:Y:2598:C:N4	23:Y:2599:G:O6	2.43	0.52
13:M:14:ARG:NH1	13:M:16:GLU:OE2	2.39	0.52
23:Y:891:G:N2	23:Y:2465:A:OP1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:GLU:OE2	3:C:58:ARG:NH1	2.43	0.51
23:Y:391:G:N7	23:Y:412:A:N6	2.58	0.51
23:Y:551:G:O2'	23:Y:553:G:O6	2.28	0.51
23:Y:2820:U:C2'	23:Y:2821:G:O5'	2.58	0.51
48:v:31:LEU:HD11	48:v:103:LEU:HD12	1.90	0.51
1:A:485:G:HO2'	1:A:486:G:P	2.30	0.51
23:Y:543:U:O2'	23:Y:544:U:OP1	2.27	0.51
35:j:55:ALA:HB2	35:j:79:LEU:HD21	1.91	0.51
7:G:42:ILE:HG21	7:G:116:MET:HE1	1.92	0.51
1:A:275:G:P	17:Q:31:LYS:HZ3	2.33	0.51
14:N:53:LEU:C	14:N:53:LEU:HD23	2.35	0.51
23:Y:945:G:N3	23:Y:2672:A:N6	2.59	0.51
43:r:39:GLY:HA3	43:r:99:VAL:HG22	1.92	0.51
7:G:27:VAL:HG12	7:G:43:VAL:HG21	1.92	0.51
49:w:50:VAL:HG22	49:w:50:VAL:O	2.11	0.51
23:Y:357:U:H1'	23:Y:358:G:OP2	2.10	0.51
24:U:15:U:OP2	24:U:71:C:O2'	2.29	0.51
13:M:4:LEU:HD21	13:M:53:VAL:HG12	1.92	0.51
21:V:192:ASP:HB3	21:V:195:VAL:HG23	1.91	0.51
23:Y:2063:G:O6	23:Y:2064:A:N6	2.44	0.51
23:Y:2702:A:OP2	54:2:2:LYS:NZ	2.35	0.51
23:Y:2788:A:O2'	23:Y:2789:A:O4'	2.23	0.51
1:A:698:A:O5'	11:K:128:ASN:ND2	2.44	0.51
18:R:18:ARG:HA	18:R:18:ARG:NE	2.26	0.51
18:R:71:ALA:HA	18:R:74:VAL:HG12	1.93	0.51
23:Y:2883:G:N2	23:Y:2886:A:OP2	2.43	0.51
1:A:275:G:O5'	17:Q:31:LYS:NZ	2.44	0.51
4:D:63:MET:HE3	4:D:64:GLU:OE1	2.10	0.51
23:Y:191:G:O2'	23:Y:917:A:N3	2.42	0.51
23:Y:2591:G:C2	23:Y:2592:C:C5	2.99	0.51
23:Y:2971:G:H21	23:Y:2981:A:H62	1.58	0.51
27:b:52:THR:HG22	27:b:93:PRO:O	2.10	0.51
1:A:884:G:OP1	2:B:18:ARG:NH2	2.42	0.50
23:Y:2819:G:N1	23:Y:2823:G:C6	2.80	0.50
23:Y:2926:A:OP2	35:j:73:LYS:NZ	2.38	0.50
25:Z:166:LEU:HD11	25:Z:176:ARG:HG2	1.93	0.50
35:j:10:LEU:HD21	35:j:40:LYS:HG2	1.92	0.50
37:l:14:ASP:O	37:l:15:ASP:OD1	2.28	0.50
1:A:735:G:OP1	15:O:65:ARG:NH2	2.38	0.50
7:G:50:ALA:O	7:G:54:THR:HG22	2.12	0.50
23:Y:682:A:OP1	27:b:96:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:U:OP2	1:A:1304:C:O2'	2.19	0.50
3:C:111:GLN:OE1	3:C:112:ALA:N	2.45	0.50
23:Y:2035:U:OP2	25:Z:157:ARG:NE	2.41	0.50
21:V:209:SER:O	21:V:213:LEU:HD23	2.12	0.50
1:A:562:U:OP2	1:A:738:G:N1	2.44	0.50
1:A:1302:C:O2	19:S:36:ARG:NH2	2.45	0.50
13:M:94:ARG:NH2	19:S:80:PHE:O	2.43	0.50
21:V:83:GLU:OE1	21:V:214:THR:OG1	2.26	0.50
23:Y:296:A:N1	23:Y:340:A:N6	2.59	0.50
23:Y:2801:A:O4'	23:Y:2836:C:N4	2.44	0.50
23:Y:1162:G:O2'	23:Y:1229:A:N6	2.45	0.50
23:Y:2087:C:N4	23:Y:2094:G:O6	2.45	0.50
23:Y:2088:C:O2'	23:Y:2089:C:C6	2.60	0.50
23:Y:2815:C:N4	23:Y:2816:G:O6	2.45	0.50
1:A:1391:A:C2	1:A:1392:C:C5	2.99	0.50
23:Y:566:A:H62	23:Y:568:A:N6	2.10	0.50
1:A:800:U:H4'	1:A:801:G:OP2	2.10	0.50
9:I:101:LEU:O	9:I:101:LEU:HD23	2.12	0.50
23:Y:2682:G:H21	23:Y:2683:A:N6	2.10	0.50
23:Y:3022:G:H2'	23:Y:3023:G:O4'	2.12	0.50
27:b:52:THR:HG21	27:b:92:GLY:HA3	1.94	0.49
29:d:35:LEU:HD11	29:d:72:LEU:CD2	2.41	0.49
1:A:178:A:H61	1:A:208:G:H3'	1.77	0.49
1:A:452:A:O2'	1:A:453:G:OP1	2.29	0.49
7:G:12:LEU:HD23	7:G:13:VAL:O	2.12	0.49
21:V:162:TRP:CH2	21:V:214:THR:HG22	2.45	0.49
23:Y:329:U:O2	23:Y:447:A:N6	2.45	0.49
23:Y:1233:A:H2'	23:Y:1234:U:N1	2.27	0.49
23:Y:2747:G:O2'	23:Y:2988:A:O2'	2.27	0.49
3:C:81:THR:O	3:C:84:ASP:OD1	2.30	0.49
4:D:147:THR:HG22	4:D:149:PRO:HD2	1.93	0.49
28:c:166:THR:HG22	28:c:166:THR:O	2.12	0.49
42:q:63:GLU:OE1	42:q:63:GLU:N	2.44	0.49
1:A:1036:U:OP1	3:C:163:SER:OG	2.29	0.49
1:A:1104:G:O2'	1:A:1126:G:N1	2.43	0.49
1:A:1248:U:O4	1:A:1309:C:O2'	2.29	0.49
23:Y:2558:C:N3	44:s:73:ARG:NH2	2.61	0.49
26:a:57:ILE:HD11	26:a:79:ARG:NE	2.27	0.49
36:k:9:ASN:OD1	36:k:10:ILE:N	2.45	0.49
18:R:18:ARG:HA	18:R:18:ARG:HE	1.77	0.49
23:Y:2536:U:OP2	28:c:78:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:2772:G:O6	23:Y:2785:A:N6	2.45	0.49
27:b:19:GLU:OE2	27:b:19:GLU:HA	2.13	0.49
53:1:31:HIS:ND1	53:1:32:LEU:HD13	2.28	0.49
23:Y:640:G:O2'	23:Y:642:G:OP2	2.30	0.49
1:A:963:U:OP2	1:A:964:U:O2'	2.23	0.49
9:I:108:ILE:HD12	9:I:115:ARG:HA	1.94	0.49
21:V:187:LEU:HD12	21:V:199:PRO:HB3	1.95	0.49
23:Y:3046:C:O4'	23:Y:3046:C:O2	2.31	0.49
30:e:110:ILE:HG23	30:e:130:ILE:HD13	1.95	0.49
35:j:65:GLU:HA	35:j:65:GLU:OE2	2.13	0.49
1:A:380:G:N1	1:A:384:G:O6	2.46	0.49
1:A:995:A:N6	1:A:1001:G:O6	2.45	0.49
4:D:87:ARG:HD3	4:D:180:LEU:HD22	1.94	0.49
21:V:152:ARG:O	21:V:155:GLN:NE2	2.43	0.49
23:Y:2653:G:N7	33:h:55:MET:HE2	2.28	0.49
25:Z:115:ASP:OD1	25:Z:116:VAL:N	2.46	0.49
1:A:457:A:O2'	1:A:458:A:O4'	2.31	0.49
1:A:735:G:P	15:O:65:ARG:HH12	2.36	0.49
1:A:965:A:O2'	1:A:1030:G:OP2	2.30	0.49
9:I:138:LEU:HD22	9:I:145:PRO:HD2	1.95	0.49
13:M:63:ASN:C	13:M:64:LEU:HD12	2.38	0.49
13:M:70:LEU:O	13:M:74:VAL:HG23	2.13	0.49
28:c:43:VAL:HG22	28:c:161:ILE:HG22	1.95	0.49
1:A:519:A:OP1	12:L:111:LYS:NZ	2.43	0.48
12:L:39:THR:HG21	12:L:49:LEU:HD11	1.94	0.48
21:V:20:THR:HG22	21:V:20:THR:O	2.12	0.48
23:Y:2764:C:O2'	23:Y:2964:A:N3	2.45	0.48
36:k:74:ASP:OD1	36:k:74:ASP:C	2.56	0.48
1:A:953:G:HO2'	1:A:1348:G:HO2'	1.40	0.48
3:C:47:GLU:N	3:C:47:GLU:OE1	2.46	0.48
5:E:174:ARG:NH1	5:E:177:GLU:OE1	2.35	0.48
9:I:63:VAL:O	9:I:67:LEU:HD23	2.13	0.48
13:M:51:ASP:OD1	13:M:51:ASP:N	2.44	0.48
23:Y:80:G:OP1	42:q:94:LYS:NZ	2.38	0.48
23:Y:1514:C:C2	23:Y:1515:C:C5	3.01	0.48
23:Y:2511:A:N7	23:Y:2513:G:C8	2.81	0.48
23:Y:2805:G:N2	23:Y:2805:G:OP2	2.46	0.48
35:j:103:ARG:NH2	35:j:106:ASP:OD2	2.45	0.48
1:A:136:G:N1	1:A:225:G:N7	2.61	0.48
23:Y:2074:G:H21	23:Y:2109:A:H62	1.60	0.48
46:u:32:LEU:HD22	46:u:46:ARG:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:U:OP2	1:A:1204:C:O2'	2.26	0.48
23:Y:298:G:N2	23:Y:338:C:N3	2.61	0.48
23:Y:1092:G:O4'	23:Y:1301:G:N2	2.47	0.48
23:Y:2130:G:H2'	23:Y:2131:G:O4'	2.13	0.48
29:d:41:ILE:HD12	29:d:65:LEU:HB3	1.96	0.48
45:t:39:VAL:HG22	45:t:46:LYS:HD3	1.95	0.48
1:A:231:G:C2	1:A:232:G:C8	3.01	0.48
4:D:105:THR:HG22	4:D:107:ARG:H	1.77	0.48
1:A:1425:G:OP2	1:A:1426:C:N4	2.45	0.48
3:C:184:TYR:OH	3:C:199:LYS:NZ	2.34	0.48
11:K:70:PHE:O	11:K:74:LEU:HD23	2.13	0.48
11:K:110:GLN:NE2	11:K:116:VAL:HG22	2.28	0.48
23:Y:989:G:O2'	34:i:65:TRP:NE1	2.44	0.48
23:Y:2851:G:N2	23:Y:3001:G:N3	2.62	0.48
1:A:1446:C:N3	1:A:1447:C:C5	2.81	0.48
11:K:125:GLN:OE1	11:K:125:GLN:HA	2.13	0.48
14:N:4:LYS:HA	14:N:7:VAL:HG12	1.95	0.48
23:Y:696:A:H2	23:Y:719:G:H21	1.62	0.48
28:c:130:ASP:OD1	28:c:132:THR:HG22	2.14	0.48
40:o:71:LEU:HD23	40:o:116:SER:HB2	1.95	0.48
1:A:363:A:OP1	12:L:31:ARG:N	2.45	0.48
1:A:565:G:H2'	1:A:566:U:O4'	2.14	0.48
1:A:806:C:O2	8:H:16:ASN:ND2	2.46	0.48
23:Y:159:A:N3	23:Y:2431:C:O2'	2.46	0.48
23:Y:755:A:C6	23:Y:756:A:N6	2.82	0.48
23:Y:1231:U:O2'	23:Y:1232:G:OP1	2.26	0.48
23:Y:2166:C:C2'	23:Y:2167:U:OP1	2.61	0.48
43:r:43:ASP:OD1	43:r:43:ASP:N	2.43	0.48
1:A:545:U:OP2	1:A:546:G:O2'	2.30	0.48
1:A:1043:C:OP2	1:A:1044:G:O2'	2.08	0.48
11:K:44:THR:OG1	11:K:49:ASN:O	2.19	0.48
12:L:14:ASP:OD1	12:L:15:LYS:N	2.47	0.48
10:J:63:GLU:OE2	14:N:45:ARG:NH2	2.47	0.47
13:M:22:ILE:HG23	13:M:67:GLU:OE2	2.14	0.47
31:f:106:ILE:HD12	31:f:119:GLN:OE1	2.14	0.47
39:n:24:VAL:HG22	39:n:25:GLU:N	2.29	0.47
41:p:26:ASP:OD1	41:p:26:ASP:O	2.32	0.47
1:A:358:U:O2	1:A:359:G:C8	2.67	0.47
23:Y:671:G:C2	23:Y:1377:A:C5	3.02	0.47
23:Y:1326:G:N2	23:Y:1351:G:O2'	2.47	0.47
32:g:45:ASP:OD1	32:g:46:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:THR:HG21	3:C:75:VAL:HG21	1.96	0.47
13:M:19:LEU:HD23	13:M:30:SER:HA	1.96	0.47
32:g:5:GLU:HA	32:g:20:LEU:HD11	1.96	0.47
2:B:24:THR:O	2:B:24:THR:HG22	2.13	0.47
4:D:83:ASP:OD1	4:D:84:ASN:N	2.47	0.47
5:E:35:ASN:OD1	5:E:35:ASN:O	2.32	0.47
23:Y:114:G:OP2	23:Y:116:A:O2'	2.32	0.47
24:U:49:C:N3	24:U:50:C:C5	2.83	0.47
26:a:114:VAL:HG11	26:a:198:ILE:HB	1.95	0.47
1:A:1291:G:N1	1:A:1310:C:N3	2.44	0.47
6:F:1:MET:HE3	6:F:1:MET:HA	1.95	0.47
15:O:71:ALA:HB2	15:O:78:TYR:CD2	2.49	0.47
21:V:221:VAL:O	21:V:225:LEU:HG	2.15	0.47
23:Y:1387:A:H62	23:Y:1836:A:H1'	1.80	0.47
29:d:35:LEU:HD23	29:d:36:ASP:N	2.29	0.47
1:A:332:G:C2	1:A:333:C:C6	3.02	0.47
17:Q:90:LEU:C	17:Q:90:LEU:HD23	2.40	0.47
23:Y:312:G:N3	23:Y:312:G:H2'	2.30	0.47
23:Y:1442:A:H2'	23:Y:1443:G:O4'	2.14	0.47
1:A:193:C:O3'	17:Q:89:ARG:NH2	2.48	0.47
7:G:27:VAL:HA	7:G:30:VAL:HG12	1.97	0.47
13:M:106:ASN:O	13:M:107:ALA:HB3	2.15	0.47
23:Y:380:A:N1	23:Y:404:A:O2'	2.27	0.47
23:Y:838:G:C2	23:Y:839:U:C4	3.03	0.47
23:Y:1433:G:H2'	23:Y:1434:G:C8	2.50	0.47
25:Z:109:GLN:N	25:Z:195:GLU:O	2.29	0.47
26:a:28:VAL:HG22	26:a:193:LEU:CD2	2.44	0.47
32:g:105:GLU:OE1	32:g:105:GLU:N	2.47	0.47
35:j:70:ILE:HD11	35:j:76:VAL:HG12	1.97	0.47
42:q:24:LEU:HD11	42:q:36:GLU:HB3	1.96	0.47
43:r:182:VAL:HG22	43:r:183:GLU:N	2.30	0.47
3:C:140:ALA:O	3:C:146:VAL:HG11	2.15	0.47
4:D:44:SER:O	4:D:48:GLN:OE1	2.32	0.47
15:O:54:ARG:HE	15:O:58:LEU:HD21	1.79	0.47
23:Y:2015:U:O2'	23:Y:2019:A:N3	2.45	0.47
23:Y:2812:G:H2'	23:Y:2813:A:O4'	2.14	0.47
1:A:260:G:N2	1:A:267:C:N3	2.62	0.47
14:N:47:MET:HA	14:N:47:MET:HE3	1.97	0.47
23:Y:3008:C:HO2'	23:Y:3009:U:P	2.38	0.47
1:A:264:U:O2'	17:Q:80:ARG:NH1	2.48	0.47
1:A:1338:G:H2'	1:A:1339:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:34:ASP:O	18:R:38:LEU:HD23	2.15	0.47
23:Y:389:G:N1	23:Y:392:A:OP2	2.45	0.47
23:Y:1102:G:OP1	23:Y:1103:C:N4	2.46	0.47
27:b:97:ASP:OD1	27:b:98:TYR:N	2.47	0.47
37:l:2:ASN:O	37:l:5:ASP:N	2.47	0.47
4:D:96:VAL:HG13	4:D:166:LEU:HD21	1.96	0.46
21:V:89:MET:SD	21:V:90:PRO:HD2	2.55	0.46
23:Y:958:A:C6	23:Y:1053:G:C6	3.03	0.46
23:Y:959:U:H2'	23:Y:960:G:O4'	2.15	0.46
23:Y:1513:C:C2	23:Y:1514:C:C5	3.03	0.46
23:Y:1874:C:OP1	26:a:146:ARG:NH1	2.47	0.46
27:b:6:ASP:OD2	27:b:6:ASP:N	2.47	0.46
36:k:37:ARG:NH2	36:k:54:ASP:OD1	2.47	0.46
23:Y:2056:G:C5	23:Y:2151:A:C2	3.04	0.46
23:Y:1982:G:O6	23:Y:2212:A:N6	2.48	0.46
23:Y:2709:G:OP1	34:i:46:GLN:NE2	2.48	0.46
31:f:14:SER:OG	31:f:52:ASP:OD2	2.33	0.46
1:A:850:C:H2'	1:A:851:A:O4'	2.15	0.46
4:D:148:LEU:O	4:D:152:ILE:HD12	2.16	0.46
19:S:10:PHE:O	19:S:39:THR:HG22	2.13	0.46
43:r:33:VAL:HG23	43:r:33:VAL:O	2.16	0.46
2:B:4:VAL:HG12	2:B:4:VAL:O	2.16	0.46
4:D:119:LEU:HD23	4:D:141:LYS:HB3	1.97	0.46
5:E:171:LEU:O	5:E:171:LEU:HD23	2.15	0.46
21:V:206:ALA:HB3	21:V:209:SER:OG	2.16	0.46
23:Y:975:U:O4	23:Y:1032:A:N7	2.48	0.46
23:Y:1106:A:C8	49:w:13:ILE:HD11	2.51	0.46
23:Y:1221:A:N7	23:Y:1222:C:N4	2.63	0.46
28:c:141:GLU:O	28:c:144:MET:HE3	2.16	0.46
6:F:30:ILE:HD11	6:F:75:LEU:HB2	1.98	0.46
9:I:61:ASN:O	9:I:65:GLN:OE1	2.33	0.46
20:T:24:VAL:O	20:T:28:LEU:HD23	2.16	0.46
20:T:47:ALA:O	20:T:48:SER:C	2.59	0.46
23:Y:1456:G:OP2	23:Y:1509:U:O2'	2.30	0.46
26:a:110:ALA:O	26:a:182:VAL:HG12	2.15	0.46
1:A:1207:C:C4	13:M:104:LYS:NZ	2.84	0.46
23:Y:24:G:O2'	23:Y:599:G:N2	2.48	0.46
23:Y:79:G:H22	23:Y:102:C:H42	1.62	0.46
23:Y:784:G:N1	23:Y:916:G:C6	2.83	0.46
23:Y:1331:C:P	38:m:15:ARG:HH12	2.39	0.46
23:Y:1378:U:C2'	23:Y:1379:G:O5'	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:1938:G:H21	23:Y:1956:A:H62	1.62	0.46
25:Z:59:LYS:O	25:Z:60:ARG:NH2	2.49	0.46
41:p:14:PRO:HD3	46:u:34:PHE:CD1	2.51	0.46
23:Y:189:A:N6	23:Y:206:A:C4	2.84	0.46
23:Y:316:U:HO2'	23:Y:317:G:P	2.31	0.46
23:Y:829:U:O2'	23:Y:831:A:N7	2.41	0.46
23:Y:1130:C:O2	31:f:27:ARG:NH1	2.49	0.46
23:Y:1146:A:N3	23:Y:2710:G:O2'	2.48	0.46
23:Y:2176:A:H2	32:g:22:ILE:HG23	1.81	0.46
24:U:47:A:C5	24:U:48:C:C5	3.04	0.46
28:c:53:ASP:OD1	28:c:53:ASP:O	2.34	0.46
12:L:76:GLU:OE1	12:L:77:HIS:ND1	2.48	0.46
23:Y:787:C:H2'	23:Y:788:C:O4'	2.16	0.46
23:Y:1688:G:C6	23:Y:1748:A:C2	3.04	0.46
23:Y:2865:G:OP2	31:f:76:ARG:NH1	2.49	0.46
1:A:653:G:H2'	1:A:654:G:C8	2.51	0.46
5:E:169:LEU:HA	5:E:172:LEU:HD23	1.98	0.46
16:P:99:LYS:HD2	16:P:100:PRO:HD2	1.97	0.46
21:V:57:VAL:O	21:V:61:VAL:HG23	2.15	0.46
23:Y:389:G:C5	23:Y:391:G:OP2	2.69	0.46
23:Y:1289:A:H2'	23:Y:1290:C:O4'	2.15	0.46
30:e:56:ILE:HD12	30:e:57:PRO:HD2	1.98	0.46
37:l:3:THR:HG23	37:l:4:LEU:HD22	1.98	0.46
1:A:664:U:O2	11:K:50:VAL:HG12	2.15	0.45
27:b:169:VAL:HG22	27:b:169:VAL:O	2.16	0.45
34:i:118:LEU:O	34:i:122:ILE:HG12	2.17	0.45
1:A:519:A:OP2	12:L:112:GLN:NE2	2.49	0.45
1:A:917:A:N1	7:G:3:ARG:NH2	2.64	0.45
1:A:1058:U:HO2'	1:A:1059:G:P	2.29	0.45
4:D:165:TRP:CD1	4:D:166:LEU:HG	2.51	0.45
23:Y:192:U:N3	23:Y:202:C:O2	2.48	0.45
23:Y:1634:C:HO2'	23:Y:1635:A:P	2.32	0.45
23:Y:2643:U:OP2	53:1:33:LEU:HD23	2.15	0.45
1:A:907:G:C2	1:A:909:G:C8	3.05	0.45
1:A:954:C:O3'	10:J:59:LYS:NZ	2.41	0.45
23:Y:2580:G:C2'	23:Y:2581:G:O4'	2.64	0.45
38:m:77:ASN:OD1	38:m:78:ARG:N	2.48	0.45
1:A:717:C:C2	1:A:718:U:C5	3.05	0.45
23:Y:1329:G:C6	23:Y:1350:G:N2	2.84	0.45
23:Y:1786:G:O2'	23:Y:1787:A:O5'	2.34	0.45
23:Y:2088:C:H1'	23:Y:2089:C:OP1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:2106:A:H3'	23:Y:2107:G:H5''	1.99	0.45
23:Y:2186:C:O2'	23:Y:2188:G:OP2	2.33	0.45
28:c:8:LEU:HD23	28:c:9:PRO:O	2.17	0.45
41:p:50:PHE:O	41:p:52:VAL:HG23	2.16	0.45
12:L:39:THR:OG1	12:L:50:ARG:O	2.23	0.45
24:U:48:C:C4	24:U:49:C:C5	3.04	0.45
28:c:111:ILE:HD12	28:c:115:LEU:HD12	1.99	0.45
30:e:137:MET:HA	30:e:137:MET:HE2	1.98	0.45
32:g:87:ILE:HD11	32:g:91:ASN:HA	1.97	0.45
1:A:175:A:OP1	20:T:56:ARG:NH2	2.48	0.45
1:A:253:U:N3	1:A:254:G:N7	2.64	0.45
1:A:859:C:C2	1:A:860:C:C5	3.05	0.45
21:V:173:VAL:O	21:V:177:ARG:HG2	2.16	0.45
24:U:44:C:O2	28:c:99:ARG:NE	2.49	0.45
30:e:121:ASN:O	30:e:122:ASP:N	2.49	0.45
1:A:72:G:N2	1:A:149:A:O2'	2.50	0.45
1:A:517:G:OP1	12:L:110:ARG:NH2	2.50	0.45
1:A:1497:A:H2'	1:A:1498:C:C6	2.52	0.45
4:D:151:GLN:O	4:D:152:ILE:C	2.58	0.45
7:G:65:ALA:O	7:G:69:VAL:HG22	2.16	0.45
9:I:72:LEU:HD11	9:I:78:VAL:HA	1.99	0.45
20:T:66:VAL:HG13	20:T:67:ILE:HG23	1.99	0.45
23:Y:433:C:O2	23:Y:433:C:H2'	2.16	0.45
23:Y:1350:G:O2'	23:Y:1351:G:O4'	2.35	0.45
24:U:33:C:C2	24:U:52:G:N2	2.85	0.45
1:A:236:G:O3'	17:Q:57:LYS:NZ	2.50	0.45
1:A:1205:U:HO2'	1:A:1206:U:P	2.37	0.45
5:E:113:GLU:HG2	5:E:118:VAL:HG22	1.97	0.45
7:G:15:ASP:OD2	7:G:17:VAL:N	2.47	0.45
17:Q:42:ASP:OD1	17:Q:42:ASP:C	2.59	0.45
23:Y:22:U:H2'	23:Y:23:G:O5'	2.17	0.45
23:Y:974:G:HO2'	23:Y:975:U:P	2.39	0.45
23:Y:2097:G:C2	23:Y:2098:U:C5	3.04	0.45
23:Y:981:U:O2'	23:Y:982:A:P	2.73	0.45
23:Y:1399:A:H2'	23:Y:1400:G:O4'	2.16	0.45
23:Y:2599:G:N2	23:Y:2602:A:OP2	2.44	0.45
23:Y:2629:G:O2'	23:Y:2630:A:OP1	2.31	0.45
23:Y:2927:C:C2	23:Y:2928:C:C5	3.05	0.45
26:a:13:MET:SD	26:a:27:THR:OG1	2.75	0.45
26:a:42:THR:HG23	26:a:43:GLU:N	2.32	0.45
33:h:135:GLU:OE2	33:h:135:GLU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1439:G:H2'	1:A:1440:A:O4'	2.16	0.45
3:C:38:ILE:O	3:C:42:LEU:HD13	2.17	0.45
3:C:58:ARG:HG3	3:C:63:VAL:HG12	1.98	0.45
4:D:118:PHE:O	4:D:119:LEU:HD22	2.16	0.45
4:D:194:LEU:HD12	4:D:194:LEU:H	1.82	0.45
10:J:57:LYS:O	10:J:58:TYR:HB2	2.16	0.45
10:J:67:MET:HE1	14:N:36:LYS:NZ	2.31	0.45
23:Y:719:G:H2'	23:Y:720:C:O4'	2.17	0.45
23:Y:808:A:N6	23:Y:885:G:O6	2.50	0.45
48:v:115:LEU:H	48:v:115:LEU:HD23	1.81	0.45
52:z:36:ASN:OD1	52:z:36:ASN:C	2.60	0.45
1:A:643:A:H2'	1:A:644:G:O4'	2.17	0.44
1:A:1232:A:N7	1:A:1268:C:N3	2.65	0.44
3:C:102:ILE:C	3:C:103:LEU:HD22	2.42	0.44
21:V:133:GLU:O	21:V:137:LEU:HD13	2.17	0.44
23:Y:1882:A:C2	23:Y:1883:A:C5	3.05	0.44
23:Y:2047:C:H2'	23:Y:2048:G:H8	1.82	0.44
23:Y:2784:C:N4	23:Y:2785:A:H62	2.15	0.44
25:Z:266:LYS:C	25:Z:267:LEU:HD22	2.43	0.44
1:A:1058:U:HO2'	1:A:1059:G:C5'	2.19	0.44
1:A:1209:C:OP2	13:M:111:LYS:NZ	2.49	0.44
1:A:1298:G:O2'	1:A:1300:A:N7	2.33	0.44
23:Y:1938:G:HO2'	23:Y:1939:U:H6	1.64	0.44
23:Y:1991:C:H2'	23:Y:1991:C:O2	2.16	0.44
23:Y:2048:G:C6	23:Y:2049:C:N4	2.85	0.44
23:Y:2800:G:H21	23:Y:2800:G:P	2.39	0.44
10:J:52:ILE:HG22	14:N:41:ARG:HD2	1.99	0.44
12:L:21:THR:HG22	12:L:24:LEU:HG	2.00	0.44
23:Y:287:A:N6	23:Y:299:G:HO2'	2.11	0.44
28:c:57:ILE:HG22	28:c:61:ILE:HD11	1.99	0.44
36:k:69:ASP:OD2	36:k:69:ASP:C	2.60	0.44
43:r:140:ILE:O	43:r:140:ILE:HG13	2.17	0.44
43:r:163:SER:C	43:r:164:LEU:HD12	2.42	0.44
23:Y:125:C:O2'	23:Y:126:C:OP2	2.29	0.44
23:Y:1089:C:O2'	23:Y:1101:A:N3	2.49	0.44
23:Y:1311:C:C2	23:Y:1312:G:C8	3.06	0.44
23:Y:1436:C:O2'	23:Y:1437:A:OP1	2.27	0.44
23:Y:1720:G:H21	25:Z:100:GLY:HA3	1.83	0.44
23:Y:2074:G:H21	23:Y:2109:A:N6	2.16	0.44
23:Y:2149:C:H2'	23:Y:2150:U:C6	2.53	0.44
23:Y:2244:A:N6	23:Y:2259:G:O6	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:2800:G:OP2	23:Y:2800:G:N2	2.38	0.44
23:Y:2944:U:H2'	23:Y:2944:U:O2	2.18	0.44
26:a:161:PHE:O	26:a:162:LYS:C	2.59	0.44
7:G:59:VAL:O	7:G:63:LYS:HE3	2.17	0.44
18:R:40:THR:HG23	18:R:41:TYR:CD2	2.53	0.44
23:Y:1448:C:H2'	23:Y:1449:C:C6	2.53	0.44
23:Y:1876:A:N6	23:Y:2227:A:N6	2.66	0.44
23:Y:1938:G:N2	23:Y:1955:A:OP2	2.42	0.44
23:Y:2077:C:N4	23:Y:2107:G:H21	2.16	0.44
23:Y:2942:G:O2'	23:Y:3068:U:OP1	2.34	0.44
25:Z:2:GLY:O	25:Z:20:ASP:N	2.45	0.44
28:c:122:ARG:O	28:c:185:LYS:NZ	2.51	0.44
31:f:122:LEU:HD23	31:f:123:LYS:N	2.32	0.44
48:v:13:ILE:HD13	48:v:56:LEU:CD2	2.48	0.44
1:A:31:G:C6	1:A:537:G:N1	2.85	0.44
6:F:74:GLU:OE2	6:F:77:ARG:NH2	2.50	0.44
9:I:101:LEU:HD23	9:I:101:LEU:C	2.43	0.44
23:Y:846:C:C2	23:Y:847:C:C5	3.06	0.44
23:Y:1019:C:C2	23:Y:1020:A:C8	3.06	0.44
23:Y:1848:A:N6	23:Y:1855:A:H61	2.15	0.44
23:Y:2130:G:H2'	23:Y:2131:G:C8	2.53	0.44
23:Y:2148:C:H2'	23:Y:2149:C:C6	2.53	0.44
23:Y:2255:A:N3	23:Y:2679:G:O2'	2.50	0.44
24:U:49:C:C2	24:U:50:C:C5	3.05	0.44
31:f:135:GLN:OE1	31:f:135:GLN:N	2.51	0.44
38:m:49:ASP:OD1	38:m:50:ARG:N	2.51	0.44
48:v:32:THR:HG22	48:v:33:VAL:N	2.33	0.44
1:A:1199:C:H2'	1:A:1200:A:H8	1.83	0.44
4:D:169:VAL:HG21	4:D:174:ARG:NH2	2.30	0.44
5:E:41:VAL:HG21	5:E:61:LEU:HD22	1.99	0.44
7:G:38:LEU:O	7:G:38:LEU:HD23	2.17	0.44
12:L:27:SER:OG	12:L:29:GLN:O	2.31	0.44
21:V:139:ARG:O	21:V:142:ASN:OD1	2.34	0.44
23:Y:485:U:O2'	23:Y:2454:G:N2	2.50	0.44
23:Y:2206:C:C2	23:Y:2207:U:C5	3.05	0.44
29:d:23:ASN:OD1	29:d:24:LEU:N	2.50	0.44
33:h:107:ASN:OD1	33:h:107:ASN:O	2.36	0.44
46:u:6:THR:HG23	46:u:9:GLU:H	1.82	0.44
4:D:63:MET:HB3	4:D:66:GLN:OE1	2.17	0.44
7:G:38:LEU:CD2	7:G:42:ILE:HD11	2.48	0.44
13:M:57:ARG:HA	13:M:60:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:46:HIS:HD2	17:Q:53:ILE:HD11	1.83	0.44
23:Y:394:G:C2	23:Y:395:G:C8	3.06	0.44
23:Y:1135:G:O6	23:Y:1265:A:N6	2.51	0.44
23:Y:1329:G:O6	23:Y:1350:G:N2	2.51	0.44
23:Y:2074:G:H5'	23:Y:2075:G:P	2.57	0.44
24:U:48:C:C2	24:U:49:C:C6	3.06	0.44
13:M:33:ILE:O	13:M:37:THR:HG23	2.17	0.43
16:P:92:THR:HG22	16:P:92:THR:O	2.18	0.43
23:Y:28:C:O2'	23:Y:1353:G:OP1	2.32	0.43
23:Y:824:G:C6	23:Y:838:G:C6	3.06	0.43
23:Y:1848:A:N6	23:Y:1855:A:N6	2.66	0.43
23:Y:2149:C:H2'	23:Y:2150:U:C2	2.52	0.43
27:b:121:ASN:ND2	33:h:3:VAL:HG22	2.33	0.43
28:c:43:VAL:HG13	28:c:161:ILE:HG22	1.99	0.43
1:A:810:G:O2'	21:V:21:ARG:CZ	2.66	0.43
1:A:998:G:H2'	1:A:999:A:C8	2.53	0.43
23:Y:543:U:H3'	23:Y:544:U:C5'	2.48	0.43
23:Y:1787:A:H2'	25:Z:86:PRO:HG3	2.00	0.43
1:A:24:U:O2'	1:A:553:A:N6	2.51	0.43
18:R:76:LEU:C	18:R:77:LEU:HD22	2.44	0.43
21:V:6:MET:HE3	21:V:43:LEU:CD1	2.47	0.43
21:V:156:LYS:O	21:V:157:VAL:CG2	2.63	0.43
23:Y:313:G:HO2'	23:Y:314:G:C4'	2.27	0.43
23:Y:2048:G:C6	23:Y:2199:G:N1	2.87	0.43
23:Y:2087:C:H2'	23:Y:2088:C:C5	2.53	0.43
1:A:1132:U:O2'	1:A:1133:G:OP2	2.32	0.43
1:A:1447:C:O2	1:A:1448:G:C8	2.72	0.43
6:F:11:ASP:OD1	6:F:11:ASP:N	2.49	0.43
9:I:125:THR:HG23	9:I:125:THR:O	2.18	0.43
23:Y:1017:G:C5	23:Y:1018:U:C5	3.06	0.43
23:Y:1092:G:C4	23:Y:1301:G:N2	2.86	0.43
23:Y:2025:C:O2	23:Y:2025:C:O4'	2.34	0.43
23:Y:2693:A:O2'	23:Y:2694:G:OP1	2.30	0.43
23:Y:2745:C:C2	23:Y:2769:G:N2	2.86	0.43
35:j:74:ASP:OD2	35:j:74:ASP:C	2.61	0.43
1:A:372:C:N4	1:A:388:G:OP2	2.52	0.43
1:A:1219:A:N3	1:A:1219:A:H2'	2.34	0.43
4:D:109:ALA:O	4:D:113:VAL:HG23	2.19	0.43
15:O:39:LEU:HD23	15:O:43:LEU:HD13	2.00	0.43
23:Y:314:G:C8	23:Y:315:U:H5	2.36	0.43
23:Y:1234:U:H2'	23:Y:1235:U:H5'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:1896:A:C4	23:Y:1897:A:C8	3.06	0.43
23:Y:2944:U:C2	23:Y:2945:A:C8	3.06	0.43
24:U:1:G:C6	24:U:117:A:N1	2.86	0.43
1:A:208:G:OP1	20:T:56:ARG:NH1	2.52	0.43
3:C:161:GLU:O	3:C:161:GLU:HG2	2.19	0.43
8:H:76:GLY:O	8:H:77:LEU:HD12	2.18	0.43
9:I:108:ILE:HD11	9:I:118:LEU:HD23	1.99	0.43
13:M:80:ARG:O	13:M:84:ILE:HG23	2.18	0.43
23:Y:502:C:N4	23:Y:503:A:H62	2.16	0.43
23:Y:840:G:O3'	23:Y:841:G:O4'	2.37	0.43
23:Y:1033:A:H2'	23:Y:1034:U:O4'	2.19	0.43
25:Z:182:ILE:HG22	25:Z:270:ARG:HG2	2.00	0.43
25:Z:220:THR:O	25:Z:221:VAL:O	2.36	0.43
32:g:7:ARG:C	32:g:8:LEU:HD12	2.43	0.43
36:k:73:ILE:HG22	36:k:75:GLY:H	1.82	0.43
36:k:83:ARG:HA	36:k:86:GLN:OE1	2.19	0.43
1:A:503:A:N6	12:L:89:ASP:OD2	2.45	0.43
1:A:814:G:C6	1:A:835:G:C6	3.05	0.43
1:A:826:U:H4'	18:R:19:LYS:HE2	2.01	0.43
1:A:997:A:H2'	1:A:998:G:C4	2.54	0.43
4:D:162:ILE:HD12	4:D:162:ILE:H	1.83	0.43
8:H:25:VAL:HG12	8:H:27:LEU:CD1	2.49	0.43
9:I:72:LEU:HD12	9:I:72:LEU:O	2.19	0.43
12:L:30:ARG:NH1	12:L:58:THR:OG1	2.51	0.43
23:Y:193:G:C2	23:Y:201:U:O2	2.71	0.43
23:Y:1083:G:O4'	23:Y:2491:A:N6	2.51	0.43
23:Y:1786:G:N2	25:Z:214:TRP:CZ3	2.87	0.43
23:Y:1899:G:N2	23:Y:1980:G:OP2	2.37	0.43
23:Y:2942:G:H2'	23:Y:2943:A:O4'	2.18	0.43
23:Y:405:G:H2'	27:b:171:ASN:HD21	1.84	0.43
23:Y:740:A:O2'	23:Y:741:G:OP2	2.24	0.43
23:Y:1191:A:C5	23:Y:1192:G:C8	3.07	0.43
23:Y:1359:G:C2	23:Y:1360:G:C8	3.06	0.43
23:Y:2830:C:O2'	23:Y:2831:G:O5'	2.37	0.43
43:r:178:VAL:HG13	43:r:179:VAL:N	2.34	0.43
1:A:941:A:HO2'	1:A:966:C:HO2'	1.49	0.43
7:G:15:ASP:OD2	7:G:15:ASP:C	2.61	0.43
13:M:77:ASP:OD1	13:M:80:ARG:NH2	2.52	0.43
15:O:47:LYS:O	15:O:53:ARG:NH2	2.52	0.43
19:S:20:ASP:O	19:S:23:ASN:OD1	2.37	0.43
23:Y:870:G:C5	23:Y:871:A:N7	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:1493:A:HO2'	23:Y:1494:U:P	2.33	0.43
23:Y:1694:C:N3	23:Y:1695:U:C5	2.87	0.43
23:Y:2148:C:H2'	23:Y:2149:C:O4'	2.19	0.43
23:Y:2916:C:C2	23:Y:2942:G:N2	2.86	0.43
38:m:97:GLU:HA	38:m:97:GLU:OE1	2.18	0.43
1:A:392:C:C2	1:A:393:A:C8	3.07	0.43
3:C:33:LYS:HG3	3:C:34:GLU:N	2.33	0.43
3:C:84:ASP:OD1	3:C:85:ARG:N	2.52	0.43
3:C:117:GLN:OE1	3:C:117:GLN:HA	2.19	0.43
3:C:206:ASP:OD1	3:C:207:ILE:N	2.50	0.43
6:F:30:ILE:HD12	6:F:75:LEU:HD22	2.00	0.43
23:Y:25:A:H2'	23:Y:26:U:O4'	2.19	0.43
23:Y:565:A:O2'	23:Y:566:A:O4'	2.35	0.43
26:a:56:GLU:OE2	26:a:57:ILE:N	2.51	0.43
28:c:47:VAL:HG23	28:c:48:GLY:N	2.34	0.43
29:d:87:LYS:HA	29:d:133:SER:HA	2.01	0.43
32:g:3:GLN:HG2	32:g:4:GLN:N	2.34	0.43
51:y:17:VAL:HG23	51:y:18:CYS:N	2.34	0.43
4:D:43:GLU:OE2	4:D:48:GLN:NE2	2.52	0.42
6:F:23:LEU:O	6:F:27:LEU:HD13	2.19	0.42
7:G:42:ILE:CG2	7:G:116:MET:HE1	2.49	0.42
23:Y:976:A:C4	23:Y:1032:A:N6	2.87	0.42
23:Y:981:U:HO2'	23:Y:982:A:P	2.31	0.42
23:Y:1310:G:C2	23:Y:1311:C:C5	3.06	0.42
26:a:142:GLN:HA	26:a:142:GLN:OE1	2.19	0.42
1:A:90:G:C2'	1:A:91:U:O5'	2.68	0.42
1:A:928:A:O2'	1:A:1315:A:N3	2.44	0.42
1:A:1266:U:O2'	1:A:1267:U:OP1	2.34	0.42
12:L:21:THR:HG23	12:L:95:TYR:HE1	1.81	0.42
16:P:48:LEU:O	16:P:49:ILE:HD13	2.19	0.42
23:Y:643:G:C2'	23:Y:644:G:OP1	2.68	0.42
23:Y:2048:G:C5	23:Y:2199:G:N2	2.87	0.42
23:Y:2831:G:H2'	23:Y:2832:G:O4'	2.19	0.42
32:g:96:THR:O	32:g:96:THR:HG22	2.18	0.42
41:p:4:ILE:HD11	46:u:22:LEU:HD22	2.00	0.42
1:A:23:C:H2'	1:A:24:U:H6	1.83	0.42
1:A:373:A:C2	1:A:374:A:N7	2.88	0.42
5:E:81:VAL:O	5:E:85:ILE:HG12	2.18	0.42
23:Y:172:C:C2	23:Y:173:U:C5	3.06	0.42
23:Y:1937:U:H2'	23:Y:1938:G:O4'	2.19	0.42
23:Y:2079:C:C2	23:Y:2105:G:N2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:2199:G:H2'	23:Y:2200:U:O4'	2.19	0.42
23:Y:3041:C:O2'	23:Y:3042:A:OP1	2.28	0.42
35:j:45:ARG:HB2	35:j:46:PRO:HD3	2.01	0.42
41:p:25:GLU:OE2	41:p:25:GLU:HA	2.20	0.42
10:J:15:HIS:HA	10:J:18:ILE:HG22	2.01	0.42
15:O:28:GLN:O	15:O:32:LEU:HD23	2.19	0.42
23:Y:103:C:H2'	23:Y:104:G:H8	1.85	0.42
23:Y:3106:C:C5	50:x:48:ARG:NH2	2.87	0.42
32:g:115:VAL:HG23	32:g:121:VAL:HG21	2.00	0.42
39:n:24:VAL:CG1	39:n:97:LEU:HD13	2.49	0.42
1:A:410:G:H21	1:A:432:A:H62	1.68	0.42
1:A:949:C:OP2	1:A:950:A:O2'	2.36	0.42
10:J:57:LYS:HG3	10:J:58:TYR:N	2.35	0.42
18:R:72:ARG:HB3	18:R:79:PHE:HE1	1.84	0.42
25:Z:166:LEU:N	25:Z:166:LEU:HD12	2.34	0.42
26:a:28:VAL:HG13	26:a:191:VAL:CG1	2.49	0.42
34:i:27:VAL:HG13	34:i:27:VAL:O	2.19	0.42
39:n:28:ASP:OD1	39:n:28:ASP:C	2.62	0.42
45:t:39:VAL:HG21	45:t:64:ALA:N	2.35	0.42
1:A:333:C:OP1	20:T:2:ALA:N	2.53	0.42
1:A:668:G:C6	1:A:680:G:C6	3.07	0.42
1:A:895:A:H4'	1:A:896:A:O5'	2.20	0.42
3:C:17:GLU:HA	3:C:17:GLU:OE2	2.20	0.42
7:G:30:VAL:HG22	7:G:30:VAL:O	2.19	0.42
16:P:15:ASN:OD1	16:P:15:ASN:O	2.37	0.42
23:Y:857:U:H2'	23:Y:858:A:C8	2.55	0.42
23:Y:1406:U:C2	23:Y:1407:G:C8	3.08	0.42
23:Y:1853:A:H2'	23:Y:1854:U:O4'	2.19	0.42
23:Y:2166:C:H3'	23:Y:2167:U:H2'	2.02	0.42
23:Y:2945:A:C4	23:Y:2946:G:C8	3.08	0.42
36:k:81:SER:O	36:k:84:VAL:HG12	2.19	0.42
50:x:35:GLN:N	50:x:35:GLN:OE1	2.52	0.42
1:A:103:G:N7	20:T:10:ARG:NH2	2.67	0.42
20:T:83:LEU:C	20:T:83:LEU:HD23	2.44	0.42
23:Y:73:C:C2	23:Y:108:A:N1	2.88	0.42
23:Y:1092:G:OP1	23:Y:1302:G:O2'	2.34	0.42
1:A:92:A:O2'	1:A:93:C:P	2.77	0.42
1:A:415:C:O2	1:A:415:C:O4'	2.37	0.42
1:A:526:G:P	4:D:64:GLU:OE2	2.78	0.42
4:D:47:ARG:O	4:D:51:GLN:HG2	2.20	0.42
8:H:10:PHE:HD1	8:H:27:LEU:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:45:ASP:O	20:T:49:GLU:OE2	2.38	0.42
23:Y:956:G:C6	23:Y:1055:G:C6	3.08	0.42
23:Y:1087:G:H2'	23:Y:1088:U:C6	2.54	0.42
23:Y:1371:G:C2	23:Y:1372:C:C5	3.07	0.42
23:Y:1777:U:OP2	23:Y:1778:A:O2'	2.21	0.42
23:Y:2154:G:HO2'	23:Y:2155:U:P	2.43	0.42
23:Y:2623:A:N6	23:Y:2642:G:O6	2.53	0.42
36:k:82:VAL:O	36:k:86:GLN:OE1	2.38	0.42
1:A:333:C:C2	1:A:334:C:C5	3.08	0.42
1:A:1138:A:N6	1:A:1161:A:N7	2.68	0.42
4:D:165:TRP:CE3	4:D:181:PRO:HB3	2.55	0.42
11:K:51:ILE:N	11:K:51:ILE:HD12	2.35	0.42
23:Y:21:G:C2	23:Y:22:U:C5	3.08	0.42
23:Y:671:G:C5	23:Y:1377:A:N6	2.88	0.42
23:Y:2042:A:H2'	23:Y:2043:C:C6	2.55	0.42
23:Y:2131:G:H2'	23:Y:2132:U:H5'	2.02	0.42
23:Y:2691:C:O2	34:i:124:LYS:NZ	2.40	0.42
23:Y:3078:G:N2	23:Y:3081:A:OP2	2.50	0.42
31:f:43:THR:O	31:f:43:THR:HG22	2.19	0.42
40:o:52:GLU:HB2	40:o:53:PRO:HD3	2.02	0.42
50:x:26:GLY:O	50:x:27:LEU:HD22	2.20	0.42
1:A:734:C:H3'	1:A:734:C:O2	2.19	0.42
1:A:1409:A:H2	1:A:1458:G:H22	1.68	0.42
1:A:1447:C:O2	1:A:1447:C:H2'	2.19	0.42
1:A:1463:G:C2	1:A:1464:G:C8	3.08	0.42
6:F:20:ALA:HB3	6:F:21:PRO:HD3	2.02	0.42
21:V:151:ILE:HA	21:V:154:MET:CG	2.50	0.42
23:Y:724:G:N2	23:Y:727:A:OP2	2.47	0.42
23:Y:974:G:O2'	23:Y:975:U:O5'	2.36	0.42
23:Y:1016:C:C2	23:Y:1017:G:C8	3.08	0.42
23:Y:1473:G:O2'	23:Y:1474:A:O5'	2.34	0.42
23:Y:1982:G:C6	23:Y:2212:A:N6	2.87	0.42
25:Z:210:GLY:O	25:Z:214:TRP:CE3	2.73	0.42
31:f:100:VAL:HG13	31:f:101:VAL:N	2.35	0.42
43:r:136:GLU:OE2	43:r:139:SER:N	2.53	0.42
1:A:298:A:C2'	1:A:299:G:O5'	2.68	0.41
1:A:406:G:H2'	1:A:407:A:O4'	2.19	0.41
1:A:560:C:H2'	1:A:561:G:O4'	2.20	0.41
13:M:103:THR:HG22	13:M:103:THR:O	2.20	0.41
21:V:171:ILE:H	21:V:171:ILE:HD12	1.84	0.41
23:Y:21:G:C2	23:Y:22:U:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:327:U:C2	23:Y:449:G:N1	2.88	0.41
23:Y:543:U:HO2'	23:Y:544:U:P	2.43	0.41
23:Y:750:C:C2	23:Y:766:G:N2	2.87	0.41
23:Y:1018:U:O2	23:Y:1019:C:C5	2.73	0.41
23:Y:1253:C:O2'	23:Y:1254:G:OP1	2.33	0.41
23:Y:1476:G:H2'	23:Y:1477:C:H6	1.85	0.41
23:Y:2819:G:C4	23:Y:2821:G:OP2	2.73	0.41
23:Y:2867:A:C4	23:Y:2868:A:C8	3.08	0.41
25:Z:248:SER:OG	25:Z:249:PRO:CD	2.68	0.41
38:m:14:ARG:O	38:m:18:LEU:HD23	2.19	0.41
39:n:24:VAL:HG12	39:n:97:LEU:HD13	2.02	0.41
1:A:702:G:N3	1:A:702:G:H2'	2.35	0.41
4:D:77:GLN:OE1	4:D:84:ASN:ND2	2.52	0.41
5:E:182:ARG:HH21	5:E:189:VAL:HG12	1.84	0.41
15:O:83:GLU:OE1	15:O:83:GLU:HA	2.20	0.41
23:Y:2529:A:O2'	23:Y:2530:C:O5'	2.35	0.41
24:U:81:U:H2'	24:U:82:A:C8	2.55	0.41
28:c:132:THR:HG23	28:c:134:ASN:HD22	1.85	0.41
34:i:84:GLY:C	34:i:85:SER:HG	2.16	0.41
35:j:73:LYS:O	35:j:76:VAL:HG22	2.20	0.41
46:u:5:THR:OG1	46:u:21:LYS:NZ	2.52	0.41
1:A:644:G:H22	1:A:721:G:H1	1.67	0.41
1:A:1462:C:C4	1:A:1463:G:C8	3.09	0.41
21:V:166:THR:HG21	21:V:195:VAL:HG11	2.02	0.41
23:Y:193:G:H2'	23:Y:194:A:O4'	2.20	0.41
23:Y:894:U:OP1	25:Z:49:ILE:HD12	2.20	0.41
23:Y:2280:G:C6	23:Y:2801:A:C4	3.09	0.41
23:Y:2972:A:H2'	23:Y:2973:A:O4'	2.20	0.41
24:U:40:A:O2'	24:U:41:U:O4'	2.38	0.41
27:b:131:VAL:HG22	27:b:132:GLU:N	2.35	0.41
31:f:37:ARG:HG3	31:f:37:ARG:HH11	1.84	0.41
1:A:362:G:O2'	1:A:363:A:N7	2.41	0.41
1:A:1342:A:C2'	1:A:1343:G:O5'	2.67	0.41
1:A:1510:G:C6	1:A:1511:C:N4	2.88	0.41
4:D:71:TYR:HA	4:D:85:LEU:HD13	2.03	0.41
15:O:79:ARG:O	15:O:83:GLU:HG2	2.20	0.41
16:P:59:TRP:HA	16:P:62:VAL:HG12	2.02	0.41
23:Y:531:A:C5	27:b:46:ARG:HD2	2.56	0.41
23:Y:684:G:HO2'	23:Y:685:G:P	2.39	0.41
23:Y:2159:G:N2	23:Y:2188:G:C4	2.88	0.41
27:b:79:THR:O	27:b:79:THR:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:106:LEU:HD12	34:i:107:SER:N	2.35	0.41
37:l:5:ASP:OD1	37:l:6:PHE:N	2.54	0.41
1:A:40:C:H2'	1:A:41:U:O4'	2.21	0.41
1:A:407:A:O3'	4:D:108:MET:HE1	2.21	0.41
1:A:747:A:C4	1:A:748:A:C8	3.08	0.41
1:A:971:G:O6	1:A:1198:C:N4	2.54	0.41
1:A:1011:U:O2	1:A:1012:U:N3	2.53	0.41
1:A:1461:U:H2'	1:A:1462:C:C6	2.55	0.41
4:D:86:LEU:HD11	4:D:192:GLU:OE2	2.20	0.41
7:G:54:THR:HG23	7:G:56:THR:H	1.85	0.41
23:Y:445:U:O2'	23:Y:446:G:OP2	2.33	0.41
23:Y:794:G:C2	23:Y:795:G:C5	3.08	0.41
23:Y:1118:A:OP2	23:Y:1273:G:N1	2.44	0.41
23:Y:1506:U:N3	23:Y:1509:U:O4	2.54	0.41
23:Y:2475:G:OP2	34:i:82:ARG:NH1	2.54	0.41
23:Y:2803:C:C2	23:Y:2804:U:C5	3.08	0.41
23:Y:2866:A:C2	23:Y:2867:A:C8	3.08	0.41
23:Y:2995:U:C2	23:Y:2996:U:C5	3.09	0.41
41:p:8:ARG:HE	41:p:49:ILE:HD11	1.85	0.41
1:A:1310:C:OP1	13:M:28:THR:HG21	2.21	0.41
1:A:1407:U:H2'	1:A:1408:A:C8	2.54	0.41
6:F:16:GLU:O	6:F:19:VAL:HG22	2.19	0.41
12:L:31:ARG:O	12:L:58:THR:HG23	2.21	0.41
16:P:6:LYS:N	16:P:21:ILE:O	2.49	0.41
23:Y:678:A:O2'	23:Y:786:C:O2'	2.36	0.41
25:Z:59:LYS:O	25:Z:60:ARG:CZ	2.68	0.41
26:a:57:ILE:HD11	26:a:79:ARG:CZ	2.51	0.41
26:a:173:ASP:N	26:a:173:ASP:OD1	2.54	0.41
34:i:122:ILE:HD12	34:i:129:ALA:HB3	2.03	0.41
48:v:110:MET:N	48:v:110:MET:SD	2.94	0.41
1:A:485:G:H2'	1:A:486:G:C8	2.55	0.41
1:A:960:A:C2	1:A:1301:A:N3	2.88	0.41
7:G:38:LEU:HD23	7:G:38:LEU:C	2.46	0.41
8:H:11:LEU:HD22	8:H:77:LEU:HD23	2.02	0.41
10:J:86:ALA:O	10:J:90:ILE:HG13	2.20	0.41
13:M:9:LEU:HD23	13:M:10:PRO:O	2.20	0.41
23:Y:643:G:C6	23:Y:644:G:N7	2.88	0.41
23:Y:1010:U:HO2'	23:Y:1011:A:P	2.34	0.41
23:Y:1019:C:H2'	23:Y:1020:A:O4'	2.20	0.41
23:Y:1069:G:O6	23:Y:1083:G:O6	2.38	0.41
23:Y:1850:A:O2'	23:Y:1851:G:O4'	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:41:VAL:HG22	28:c:163:VAL:HG12	2.03	0.41
28:c:87:ARG:HG3	28:c:87:ARG:HH11	1.86	0.41
29:d:35:LEU:HD11	29:d:72:LEU:HD22	2.02	0.41
40:o:39:ALA:O	40:o:43:LEU:HD23	2.21	0.41
46:u:22:LEU:HD23	46:u:22:LEU:O	2.20	0.41
1:A:1303:U:O2	1:A:1303:U:O5'	2.39	0.41
15:O:79:ARG:HG3	15:O:79:ARG:HH11	1.86	0.41
23:Y:417:C:O2	42:q:69:SER:OG	2.38	0.41
23:Y:558:A:C2	23:Y:559:A:C5	3.09	0.41
23:Y:1077:A:C8	23:Y:1079:C:C6	3.08	0.41
23:Y:2802:G:C2	23:Y:2803:C:C5	3.09	0.41
33:h:57:ILE:HD12	33:h:57:ILE:H	1.85	0.41
33:h:75:TYR:CD1	33:h:109:LEU:HD23	2.56	0.41
38:m:18:LEU:HD21	38:m:32:TYR:HB2	2.02	0.41
45:t:41:ARG:HH11	45:t:41:ARG:HG2	1.86	0.41
1:A:592:U:H2'	1:A:593:C:C6	2.56	0.41
1:A:827:U:H4'	1:A:827:U:OP2	2.21	0.41
14:N:24:CYS:O	14:N:28:GLY:N	2.46	0.41
18:R:40:THR:O	18:R:49:ARG:NH2	2.54	0.41
23:Y:193:G:N1	23:Y:201:U:C2	2.88	0.41
23:Y:662:G:C1'	23:Y:1101:A:H62	2.34	0.41
23:Y:953:G:C6	23:Y:1058:A:N6	2.88	0.41
23:Y:1000:C:H2'	23:Y:1001:C:O4'	2.21	0.41
23:Y:1013:U:H3'	23:Y:1014:G:O4'	2.21	0.41
24:U:22:A:N6	24:U:64:G:O6	2.54	0.41
26:a:60:ARG:HB3	26:a:60:ARG:CZ	2.51	0.41
26:a:63:ILE:HD12	26:a:63:ILE:H	1.86	0.41
28:c:60:ALA:O	28:c:64:LEU:HD23	2.20	0.41
28:c:154:ASP:OD1	28:c:154:ASP:N	2.54	0.41
29:d:59:GLU:OE1	29:d:62:SER:N	2.50	0.41
39:n:16:VAL:HG21	39:n:99:VAL:HG11	2.03	0.41
42:q:81:THR:HG22	42:q:82:ARG:O	2.21	0.41
1:A:510:G:H2'	1:A:510:G:N3	2.35	0.41
9:I:45:THR:HG23	9:I:47:GLN:HG2	2.02	0.41
11:K:81:ARG:CZ	11:K:81:ARG:HB2	2.51	0.41
16:P:104:ASP:OD1	16:P:104:ASP:C	2.64	0.41
20:T:8:ILE:HD12	20:T:8:ILE:H	1.86	0.41
23:Y:312:G:H2'	23:Y:313:G:O5'	2.21	0.41
23:Y:857:U:H2'	23:Y:858:A:H8	1.86	0.41
23:Y:1321:C:H1'	23:Y:1355:G:H22	1.85	0.41
23:Y:1821:A:C5	23:Y:1822:C:C5	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:35:ARG:HH11	25:Z:35:ARG:HG2	1.86	0.41
39:n:41:LEU:CD2	39:n:43:VAL:HG23	2.51	0.41
1:A:311:C:N3	1:A:312:C:C5	2.89	0.40
1:A:357:G:C2	1:A:358:U:C5	3.09	0.40
1:A:596:A:C6	1:A:605:G:C6	3.09	0.40
1:A:1482:U:C2'	1:A:1483:A:OP2	2.69	0.40
9:I:55:LEU:HD12	9:I:56:GLU:N	2.36	0.40
23:Y:283:U:O2	23:Y:303:G:O6	2.39	0.40
23:Y:910:C:C2	23:Y:911:U:C5	3.08	0.40
23:Y:2014:G:C2	23:Y:2040:G:C2	3.10	0.40
27:b:160:ARG:HG2	27:b:160:ARG:HH11	1.86	0.40
54:2:10:ILE:HG23	54:2:11:CYS:N	2.37	0.40
1:A:491:C:O2'	1:A:492:U:OP2	2.34	0.40
1:A:495:G:C6	1:A:517:G:C6	3.09	0.40
1:A:995:A:C6	1:A:1001:G:C6	3.09	0.40
1:A:1448:G:C2	1:A:1449:U:C5	3.09	0.40
3:C:30:ASP:HA	3:C:33:LYS:HG2	2.04	0.40
4:D:97:VAL:CG1	4:D:109:ALA:HB1	2.51	0.40
4:D:189:PRO:O	4:D:190:LEU:HB2	2.21	0.40
5:E:196:LYS:O	5:E:200:GLU:HG3	2.21	0.40
9:I:38:ARG:O	9:I:85:ALA:HA	2.21	0.40
21:V:54:TYR:CE1	21:V:58:LYS:NZ	2.87	0.40
23:Y:684:G:H3'	23:Y:685:G:C5'	2.51	0.40
23:Y:1349:U:HO2'	23:Y:1350:G:P	2.44	0.40
23:Y:1694:C:C2	23:Y:1695:U:C5	3.09	0.40
23:Y:2945:A:C6	23:Y:2946:G:C5	3.10	0.40
23:Y:2990:A:C2	23:Y:2991:C:C6	3.10	0.40
25:Z:154:LYS:O	25:Z:154:LYS:HG2	2.21	0.40
1:A:1301:A:OP2	19:S:3:ARG:NH1	2.54	0.40
4:D:80:LYS:O	4:D:83:ASP:OD1	2.40	0.40
4:D:85:LEU:HA	4:D:88:ILE:HG22	2.03	0.40
7:G:115:THR:HG22	7:G:117:VAL:HG12	2.03	0.40
15:O:39:LEU:HD22	15:O:56:LEU:HD22	2.03	0.40
23:Y:516:G:C2'	23:Y:517:A:O5'	2.69	0.40
23:Y:1192:G:C2	23:Y:1193:C:C5	3.10	0.40
23:Y:1405:U:C2	23:Y:1406:U:C5	3.09	0.40
26:a:28:VAL:HG13	26:a:191:VAL:HG13	2.03	0.40
26:a:109:GLY:H	26:a:182:VAL:HG13	1.86	0.40
27:b:66:TYR:OH	27:b:74:ALA:O	2.35	0.40
31:f:122:LEU:HD23	31:f:122:LEU:C	2.47	0.40
54:2:27:CYS:SG	54:2:28:SER:N	2.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:G:N7	5:E:120:MET:HE1	2.36	0.40
1:A:638:A:OP1	15:O:8:LYS:NZ	2.45	0.40
1:A:1199:C:H2'	1:A:1200:A:C8	2.56	0.40
5:E:139:VAL:HG11	5:E:165:THR:HG21	2.02	0.40
21:V:33:THR:HG22	21:V:34:ASP:N	2.37	0.40
23:Y:139:U:O2	23:Y:139:U:O4'	2.39	0.40
23:Y:1377:A:N3	23:Y:1378:U:C5	2.90	0.40
28:c:47:VAL:HG21	28:c:56:LEU:HD11	2.02	0.40
29:d:74:ALA:O	29:d:77:VAL:HG12	2.22	0.40
33:h:73:THR:O	33:h:73:THR:HG23	2.21	0.40
42:q:22:LYS:O	42:q:24:LEU:HD12	2.22	0.40
43:r:75:GLU:N	43:r:75:GLU:OE2	2.54	0.40
1:A:11:G:C5	1:A:298:A:N6	2.90	0.40
1:A:746:A:C2	1:A:747:A:H1'	2.57	0.40
4:D:24:GLN:HE21	4:D:24:GLN:HB2	1.75	0.40
5:E:50:VAL:HG22	5:E:51:LYS:N	2.37	0.40
20:T:46:LYS:HA	20:T:49:GLU:OE1	2.22	0.40
23:Y:40:G:C2	23:Y:525:C:C2	3.10	0.40
23:Y:282:A:H2'	23:Y:283:U:O4'	2.22	0.40
23:Y:587:G:H21	23:Y:592:A:H62	1.69	0.40
23:Y:2093:G:O2'	23:Y:2094:G:H5''	2.21	0.40
23:Y:2180:U:C4	23:Y:2181:C:C5	3.10	0.40
23:Y:2181:C:C2	23:Y:2182:C:C5	3.10	0.40
24:U:46:A:C4	24:U:47:A:C8	3.10	0.40
27:b:67:ARG:HH11	27:b:67:ARG:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	30/33 (91%)	29 (97%)	1 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	206/275 (75%)	197 (96%)	9 (4%)	0	100	100
4	D	198/201 (98%)	184 (93%)	14 (7%)	0	100	100
5	E	178/214 (83%)	172 (97%)	6 (3%)	0	100	100
6	F	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	152 (99%)	1 (1%)	0	100	100
8	H	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
9	I	124/150 (83%)	112 (90%)	12 (10%)	0	100	100
10	J	97/101 (96%)	92 (95%)	5 (5%)	0	100	100
11	K	113/138 (82%)	106 (94%)	7 (6%)	0	100	100
12	L	120/124 (97%)	110 (92%)	10 (8%)	0	100	100
13	M	114/124 (92%)	110 (96%)	4 (4%)	0	100	100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	P	111/156 (71%)	106 (96%)	5 (4%)	0	100	100
17	Q	92/98 (94%)	89 (97%)	3 (3%)	0	100	100
18	R	63/84 (75%)	59 (94%)	4 (6%)	0	100	100
19	S	80/93 (86%)	78 (98%)	2 (2%)	0	100	100
20	T	83/86 (96%)	83 (100%)	0	0	100	100
21	V	226/277 (82%)	218 (96%)	6 (3%)	2 (1%)	14	41
25	Z	273/278 (98%)	263 (96%)	9 (3%)	1 (0%)	30	58
26	a	212/217 (98%)	196 (92%)	16 (8%)	0	100	100
27	b	207/215 (96%)	200 (97%)	7 (3%)	0	100	100
28	c	180/187 (96%)	174 (97%)	6 (3%)	0	100	100
29	d	174/179 (97%)	169 (97%)	5 (3%)	0	100	100
30	e	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
31	f	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
32	g	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
33	h	143/147 (97%)	129 (90%)	14 (10%)	0	100	100
34	i	134/138 (97%)	127 (95%)	7 (5%)	0	100	100
35	j	116/199 (58%)	107 (92%)	9 (8%)	0	100	100
36	k	124/127 (98%)	122 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	l	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
38	m	122/129 (95%)	118 (97%)	4 (3%)	0	100	100
39	n	98/103 (95%)	95 (97%)	3 (3%)	0	100	100
40	o	112/153 (73%)	107 (96%)	5 (4%)	0	100	100
41	p	95/100 (95%)	92 (97%)	3 (3%)	0	100	100
42	q	93/105 (89%)	91 (98%)	2 (2%)	0	100	100
43	r	190/215 (88%)	184 (97%)	6 (3%)	0	100	100
44	s	77/88 (88%)	74 (96%)	3 (4%)	0	100	100
45	t	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
46	u	62/77 (80%)	61 (98%)	1 (2%)	0	100	100
47	5	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
48	v	124/175 (71%)	122 (98%)	1 (1%)	1 (1%)	16	44
49	w	57/61 (93%)	54 (95%)	3 (5%)	0	100	100
50	x	52/57 (91%)	52 (100%)	0	0	100	100
51	y	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
52	z	44/47 (94%)	44 (100%)	0	0	100	100
53	1	61/64 (95%)	57 (93%)	4 (7%)	0	100	100
54	2	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	5740/6453 (89%)	5500 (96%)	236 (4%)	4 (0%)	49	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	V	155	GLN
25	Z	221	VAL
48	v	85	GLU
21	V	157	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	30/31 (97%)	30 (100%)	0	100	100
3	C	170/212 (80%)	170 (100%)	0	100	100
4	D	175/176 (99%)	174 (99%)	1 (1%)	78	81
5	E	127/147 (86%)	127 (100%)	0	100	100
6	F	85/85 (100%)	85 (100%)	0	100	100
7	G	131/132 (99%)	131 (100%)	0	100	100
8	H	107/108 (99%)	107 (100%)	0	100	100
9	I	102/125 (82%)	102 (100%)	0	100	100
10	J	89/90 (99%)	89 (100%)	0	100	100
11	K	89/105 (85%)	89 (100%)	0	100	100
12	L	103/105 (98%)	103 (100%)	0	100	100
13	M	99/104 (95%)	99 (100%)	0	100	100
14	N	49/50 (98%)	49 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	92/118 (78%)	92 (100%)	0	100	100
17	Q	80/83 (96%)	80 (100%)	0	100	100
18	R	55/72 (76%)	55 (100%)	0	100	100
19	S	73/84 (87%)	73 (100%)	0	100	100
20	T	69/70 (99%)	68 (99%)	1 (1%)	59	73
21	V	191/218 (88%)	191 (100%)	0	100	100
25	Z	215/218 (99%)	215 (100%)	0	100	100
26	a	160/163 (98%)	160 (100%)	0	100	100
27	b	169/173 (98%)	168 (99%)	1 (1%)	78	81
28	c	151/156 (97%)	150 (99%)	1 (1%)	76	80
29	d	148/150 (99%)	148 (100%)	0	100	100
30	e	102/108 (94%)	102 (100%)	0	100	100
31	f	119/120 (99%)	119 (100%)	0	100	100
32	g	100/100 (100%)	100 (100%)	0	100	100
33	h	112/114 (98%)	112 (100%)	0	100	100
34	i	114/116 (98%)	114 (100%)	0	100	100
35	j	97/158 (61%)	97 (100%)	0	100	100
36	k	93/94 (99%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	l	100/100 (100%)	100 (100%)	0	100	100
38	m	97/99 (98%)	97 (100%)	0	100	100
39	n	81/83 (98%)	81 (100%)	0	100	100
40	o	90/117 (77%)	89 (99%)	1 (1%)	65	76
41	p	83/85 (98%)	83 (100%)	0	100	100
42	q	81/86 (94%)	81 (100%)	0	100	100
43	r	155/168 (92%)	155 (100%)	0	100	100
44	s	58/63 (92%)	58 (100%)	0	100	100
45	t	50/51 (98%)	50 (100%)	0	100	100
46	u	58/66 (88%)	58 (100%)	0	100	100
47	5	18/19 (95%)	18 (100%)	0	100	100
48	v	89/120 (74%)	89 (100%)	0	100	100
49	w	52/54 (96%)	52 (100%)	0	100	100
50	x	43/46 (94%)	43 (100%)	0	100	100
51	y	47/52 (90%)	47 (100%)	0	100	100
52	z	35/36 (97%)	35 (100%)	0	100	100
53	1	53/54 (98%)	53 (100%)	0	100	100
54	2	35/35 (100%)	35 (100%)	0	100	100
All	All	4797/5196 (92%)	4792 (100%)	5 (0%)	87	89

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

Mol	Chain	Res	Type
4	D	24	GLN
20	T	84	ASN
27	b	171	ASN
28	c	140	ASN
40	o	64	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	146	ASN
7	G	86	GLN
8	H	121	GLN

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Mol	Chain	Res	Type
9	I	66	GLN
9	I	146	GLN
11	K	58	HIS
11	K	110	GLN
11	K	127	HIS
21	V	112	GLN
25	Z	96	HIS
25	Z	129	ASN
25	Z	203	ASN
25	Z	205	ASN
26	a	21	ASN
26	a	99	GLN
27	b	171	ASN
30	e	14	GLN
32	g	89	ASN
35	j	31	HIS
41	p	58	ASN
42	q	101	ASN
43	r	46	HIS
43	r	61	HIS
43	r	161	GLN
47	5	23	ASN
53	1	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1528 (98%)	292 (19%)	16 (1%)
22	X	5/6 (83%)	0	0
23	Y	2931/3120 (93%)	534 (18%)	34 (1%)
24	U	117/118 (99%)	13 (11%)	1 (0%)
All	All	4563/4772 (95%)	839 (18%)	51 (1%)

All (839) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	11	G
1	A	12	A
1	A	13	G

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Mol	Chain	Res	Type
1	A	35	G
1	A	36	A
1	A	43	G
1	A	51	C
1	A	52	U
1	A	53	U
1	A	54	A
1	A	55	A
1	A	58	C
1	A	59	A
1	A	75	A
1	A	82	U
1	A	85	C
1	A	87	G
1	A	89	G
1	A	91	U
1	A	92	A
1	A	93	C
1	A	106	C
1	A	116	A
1	A	117	C
1	A	118	A
1	A	126	G
1	A	128	U
1	A	139	C
1	A	141	U
1	A	159	A
1	A	177	U
1	A	179	C
1	A	180	A
1	A	189	G
1	A	192	G
1	A	193	C
1	A	194	A
1	A	195	U
1	A	196	G
1	A	201	G
1	A	211	A
1	A	215	U
1	A	217	U
1	A	220	G
1	A	227	G

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Mol	Chain	Res	Type
1	A	245	C
1	A	247	G
1	A	251	G
1	A	252	U
1	A	256	U
1	A	266	G
1	A	267	C
1	A	278	G
1	A	280	C
1	A	281	G
1	A	289	G
1	A	299	G
1	A	306	A
1	A	325	A
1	A	326	G
1	A	328	U
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	351	G
1	A	352	C
1	A	353	A
1	A	367	U
1	A	371	A
1	A	372	C
1	A	390	U
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	414	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	426	U
1	A	427	U
1	A	429	U
1	A	430	A
1	A	434	C
1	A	435	U

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Mol	Chain	Res	Type
1	A	438	U
1	A	439	U
1	A	452	A
1	A	453	G
1	A	454	C
1	A	456	C
1	A	457	A
1	A	458	A
1	A	459	G
1	A	465	G
1	A	466	U
1	A	469	G
1	A	477	G
1	A	485	G
1	A	486	G
1	A	489	A
1	A	491	C
1	A	492	U
1	A	496	U
1	A	498	C
1	A	499	C
1	A	507	G
1	A	511	U
1	A	512	A
1	A	513	A
1	A	515	A
1	A	519	A
1	A	520	G
1	A	527	A
1	A	539	A
1	A	542	U
1	A	544	C
1	A	553	A
1	A	556	A
1	A	557	G
1	A	601	A
1	A	612	U
1	A	613	G
1	A	633	A
1	A	645	G
1	A	666	U
1	A	668	G

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Mol	Chain	Res	Type
1	A	675	A
1	A	677	U
1	A	683	G
1	A	698	A
1	A	701	G
1	A	702	G
1	A	703	U
1	A	711	G
1	A	713	G
1	A	728	A
1	A	729	A
1	A	735	G
1	A	757	A
1	A	765	G
1	A	773	U
1	A	774	A
1	A	795	A
1	A	797	C
1	A	808	A
1	A	822	U
1	A	823	U
1	A	824	C
1	A	827	U
1	A	828	G
1	A	841	U
1	A	854	A
1	A	884	G
1	A	896	A
1	A	908	G
1	A	909	G
1	A	916	C
1	A	917	A
1	A	921	G
1	A	942	U
1	A	943	U
1	A	947	U
1	A	950	A
1	A	951	A
1	A	953	G
1	A	955	G
1	A	956	A
1	A	957	A

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Mol	Chain	Res	Type
1	A	959	A
1	A	960	A
1	A	971	G
1	A	973	U
1	A	974	U
1	A	975	G
1	A	976	A
1	A	981	C
1	A	982	A
1	A	986	G
1	A	988	C
1	A	998	G
1	A	1008	C
1	A	1010	C
1	A	1012	U
1	A	1013	G
1	A	1014	U
1	A	1024	G
1	A	1025	C
1	A	1033	G
1	A	1034	C
1	A	1036	U
1	A	1045	U
1	A	1058	U
1	A	1059	G
1	A	1074	G
1	A	1075	U
1	A	1079	G
1	A	1081	A
1	A	1104	G
1	A	1108	C
1	A	1110	A
1	A	1115	G
1	A	1116	U
1	A	1117	U
1	A	1118	A
1	A	1120	G
1	A	1121	G
1	A	1127	A
1	A	1130	C
1	A	1133	G
1	A	1138	A

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Mol	Chain	Res	Type
1	A	1140	U
1	A	1147	G
1	A	1148	U
1	A	1149	C
1	A	1150	A
1	A	1151	A
1	A	1162	G
1	A	1165	G
1	A	1172	A
1	A	1177	A
1	A	1178	A
1	A	1181	C
1	A	1182	A
1	A	1193	U
1	A	1194	A
1	A	1206	U
1	A	1207	C
1	A	1219	A
1	A	1231	A
1	A	1238	U
1	A	1239	G
1	A	1241	G
1	A	1248	U
1	A	1250	A
1	A	1251	G
1	A	1261	A
1	A	1265	U
1	A	1266	U
1	A	1267	U
1	A	1268	C
1	A	1269	A
1	A	1279	U
1	A	1282	G
1	A	1283	U
1	A	1284	U
1	A	1285	C
1	A	1287	G
1	A	1301	A
1	A	1313	G
1	A	1328	A
1	A	1329	G
1	A	1343	G

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Mol	Chain	Res	Type
1	A	1344	C
1	A	1346	A
1	A	1347	C
1	A	1351	G
1	A	1357	A
1	A	1380	C
1	A	1381	A
1	A	1382	C
1	A	1383	C
1	A	1384	G
1	A	1407	U
1	A	1411	A
1	A	1412	C
1	A	1413	C
1	A	1425	G
1	A	1429	A
1	A	1433	C
1	A	1434	U
1	A	1435	U
1	A	1436	G
1	A	1438	G
1	A	1460	A
1	A	1463	G
1	A	1475	G
1	A	1476	A
1	A	1478	G
1	A	1483	A
1	A	1487	A
1	A	1488	G
1	A	1490	U
1	A	1501	G
1	A	1502	A
1	A	1504	G
1	A	1513	G
1	A	1514	G
23	Y	7	U
23	Y	20	G
23	Y	22	U
23	Y	23	G
23	Y	31	U
23	Y	32	G
23	Y	60	A

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Mol	Chain	Res	Type
23	Y	61	G
23	Y	68	A
23	Y	71	A
23	Y	72	G
23	Y	82	G
23	Y	89	A
23	Y	90	C
23	Y	94	G
23	Y	95	C
23	Y	98	U
23	Y	99	G
23	Y	115	A
23	Y	117	U
23	Y	125	C
23	Y	126	C
23	Y	148	A
23	Y	172	C
23	Y	180	A
23	Y	189	A
23	Y	195	A
23	Y	212	A
23	Y	215	A
23	Y	220	A
23	Y	221	A
23	Y	227	A
23	Y	228	A
23	Y	229	U
23	Y	230	G
23	Y	231	U
23	Y	248	G
23	Y	272	A
23	Y	274	C
23	Y	275	C
23	Y	279	U
23	Y	282	A
23	Y	285	U
23	Y	286	G
23	Y	291	C
23	Y	296	A
23	Y	300	G
23	Y	301	U
23	Y	303	G

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Mol	Chain	Res	Type
23	Y	311	G
23	Y	313	G
23	Y	314	G
23	Y	315	U
23	Y	317	G
23	Y	318	U
23	Y	319	G
23	Y	323	C
23	Y	324	C
23	Y	330	U
23	Y	331	U
23	Y	336	C
23	Y	337	U
23	Y	338	C
23	Y	342	C
23	Y	344	G
23	Y	352	G
23	Y	355	A
23	Y	357	U
23	Y	358	G
23	Y	361	A
23	Y	367	U
23	Y	369	G
23	Y	370	U
23	Y	384	G
23	Y	389	G
23	Y	393	U
23	Y	399	G
23	Y	404	A
23	Y	405	G
23	Y	412	A
23	Y	414	A
23	Y	415	G
23	Y	420	G
23	Y	424	G
23	Y	425	U
23	Y	433	C
23	Y	434	G
23	Y	445	U
23	Y	446	G
23	Y	450	G
23	Y	452	G

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Mol	Chain	Res	Type
23	Y	453	U
23	Y	454	U
23	Y	455	C
23	Y	459	A
23	Y	460	G
23	Y	472	C
23	Y	473	C
23	Y	474	G
23	Y	475	U
23	Y	489	A
23	Y	490	A
23	Y	494	G
23	Y	498	G
23	Y	499	G
23	Y	500	A
23	Y	505	C
23	Y	512	G
23	Y	517	A
23	Y	539	C
23	Y	543	U
23	Y	544	U
23	Y	552	U
23	Y	553	G
23	Y	562	G
23	Y	568	A
23	Y	569	G
23	Y	589	A
23	Y	591	G
23	Y	592	A
23	Y	594	U
23	Y	595	A
23	Y	596	C
23	Y	597	C
23	Y	617	U
23	Y	618	C
23	Y	619	C
23	Y	620	G
23	Y	631	C
23	Y	634	C
23	Y	635	G
23	Y	636	U
23	Y	637	G

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Mol	Chain	Res	Type
23	Y	638	U
23	Y	639	C
23	Y	640	G
23	Y	642	G
23	Y	644	G
23	Y	647	G
23	Y	655	G
23	Y	658	U
23	Y	661	U
23	Y	663	A
23	Y	665	G
23	Y	667	A
23	Y	678	A
23	Y	679	G
23	Y	684	G
23	Y	685	G
23	Y	696	A
23	Y	706	G
23	Y	707	G
23	Y	708	G
23	Y	709	U
23	Y	710	G
23	Y	714	U
23	Y	721	A
23	Y	731	A
23	Y	738	A
23	Y	740	A
23	Y	747	A
23	Y	749	C
23	Y	756	A
23	Y	757	G
23	Y	758	A
23	Y	760	U
23	Y	764	U
23	Y	766	G
23	Y	768	G
23	Y	769	U
23	Y	784	G
23	Y	801	U
23	Y	828	G
23	Y	829	U
23	Y	839	U

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Mol	Chain	Res	Type
23	Y	841	G
23	Y	845	C
23	Y	862	U
23	Y	863	G
23	Y	868	C
23	Y	872	G
23	Y	879	A
23	Y	880	G
23	Y	890	G
23	Y	891	G
23	Y	897	A
23	Y	899	G
23	Y	900	G
23	Y	919	A
23	Y	920	G
23	Y	927	C
23	Y	934	A
23	Y	942	U
23	Y	960	G
23	Y	961	U
23	Y	962	U
23	Y	974	G
23	Y	975	U
23	Y	981	U
23	Y	982	A
23	Y	995	U
23	Y	998	G
23	Y	1001	C
23	Y	1003	A
23	Y	1004	C
23	Y	1005	A
23	Y	1010	U
23	Y	1011	A
23	Y	1012	C
23	Y	1014	G
23	Y	1025	A
23	Y	1032	A
23	Y	1033	A
23	Y	1034	U
23	Y	1046	C
23	Y	1047	A
23	Y	1048	A

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Mol	Chain	Res	Type
23	Y	1049	G
23	Y	1063	G
23	Y	1075	U
23	Y	1076	A
23	Y	1078	G
23	Y	1085	G
23	Y	1092	G
23	Y	1101	A
23	Y	1114	G
23	Y	1115	G
23	Y	1127	A
23	Y	1130	C
23	Y	1131	G
23	Y	1138	A
23	Y	1140	G
23	Y	1144	A
23	Y	1151	U
23	Y	1163	A
23	Y	1164	A
23	Y	1181	G
23	Y	1184	U
23	Y	1185	A
23	Y	1186	G
23	Y	1187	A
23	Y	1188	A
23	Y	1189	G
23	Y	1190	C
23	Y	1191	A
23	Y	1194	C
23	Y	1196	C
23	Y	1202	A
23	Y	1205	G
23	Y	1206	A
23	Y	1207	G
23	Y	1209	G
23	Y	1213	A
23	Y	1219	U
23	Y	1222	C
23	Y	1226	U
23	Y	1230	G
23	Y	1232	G
23	Y	1234	U

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Mol	Chain	Res	Type
23	Y	1240	G
23	Y	1251	A
23	Y	1253	C
23	Y	1260	C
23	Y	1261	A
23	Y	1262	A
23	Y	1270	G
23	Y	1274	A
23	Y	1293	G
23	Y	1298	C
23	Y	1301	G
23	Y	1341	U
23	Y	1344	A
23	Y	1350	G
23	Y	1353	G
23	Y	1371	G
23	Y	1379	G
23	Y	1384	G
23	Y	1386	G
23	Y	1387	A
23	Y	1389	U
23	Y	1415	A
23	Y	1416	A
23	Y	1436	C
23	Y	1437	A
23	Y	1448	C
23	Y	1465	C
23	Y	1474	A
23	Y	1480	A
23	Y	1493	A
23	Y	1494	U
23	Y	1499	A
23	Y	1510	A
23	Y	1511	U
23	Y	1522	G
23	Y	1531	C
23	Y	1532	G
23	Y	1533	U
23	Y	1534	C
23	Y	1540	U
23	Y	1629	G
23	Y	1631	A

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Mol	Chain	Res	Type
23	Y	1635	A
23	Y	1636	A
23	Y	1637	G
23	Y	1640	A
23	Y	1641	U
23	Y	1649	C
23	Y	1674	G
23	Y	1676	G
23	Y	1679	A
23	Y	1680	A
23	Y	1681	U
23	Y	1703	G
23	Y	1705	C
23	Y	1709	U
23	Y	1710	A
23	Y	1713	U
23	Y	1714	A
23	Y	1717	U
23	Y	1728	U
23	Y	1729	A
23	Y	1730	U
23	Y	1731	A
23	Y	1737	A
23	Y	1746	G
23	Y	1754	G
23	Y	1755	A
23	Y	1758	G
23	Y	1767	U
23	Y	1786	G
23	Y	1787	A
23	Y	1788	G
23	Y	1789	A
23	Y	1798	U
23	Y	1801	C
23	Y	1802	G
23	Y	1803	A
23	Y	1825	C
23	Y	1834	A
23	Y	1849	G
23	Y	1850	A
23	Y	1864	U
23	Y	1866	C

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Mol	Chain	Res	Type
23	Y	1870	U
23	Y	1871	G
23	Y	1872	A
23	Y	1892	G
23	Y	1912	C
23	Y	1916	A
23	Y	1917	G
23	Y	1933	G
23	Y	1946	U
23	Y	1947	U
23	Y	1950	G
23	Y	1973	C
23	Y	1975	A
23	Y	1981	U
23	Y	1990	A
23	Y	1998	C
23	Y	2001	A
23	Y	2008	A
23	Y	2017	C
23	Y	2018	G
23	Y	2025	C
23	Y	2026	A
23	Y	2033	U
23	Y	2034	G
23	Y	2036	A
23	Y	2038	A
23	Y	2047	C
23	Y	2066	G
23	Y	2074	G
23	Y	2075	G
23	Y	2083	A
23	Y	2085	C
23	Y	2086	U
23	Y	2088	C
23	Y	2089	C
23	Y	2090	U
23	Y	2091	U
23	Y	2092	U
23	Y	2093	G
23	Y	2094	G
23	Y	2095	G
23	Y	2096	G

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Mol	Chain	Res	Type
23	Y	2106	A
23	Y	2107	G
23	Y	2111	U
23	Y	2112	U
23	Y	2130	G
23	Y	2131	G
23	Y	2137	A
23	Y	2138	C
23	Y	2140	A
23	Y	2142	A
23	Y	2150	U
23	Y	2153	G
23	Y	2154	G
23	Y	2162	A
23	Y	2163	U
23	Y	2166	C
23	Y	2167	U
23	Y	2179	U
23	Y	2187	U
23	Y	2191	C
23	Y	2194	A
23	Y	2195	U
23	Y	2196	G
23	Y	2213	A
23	Y	2215	U
23	Y	2217	U
23	Y	2221	A
23	Y	2237	A
23	Y	2247	A
23	Y	2254	A
23	Y	2255	A
23	Y	2256	G
23	Y	2257	A
23	Y	2258	U
23	Y	2267	C
23	Y	2276	G
23	Y	2279	C
23	Y	2280	G
23	Y	2283	A
23	Y	2284	A
23	Y	2285	G
23	Y	2286	A

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Mol	Chain	Res	Type
23	Y	2316	G
23	Y	2320	C
23	Y	2323	G
23	Y	2408	G
23	Y	2409	U
23	Y	2411	U
23	Y	2422	A
23	Y	2427	G
23	Y	2434	A
23	Y	2436	A
23	Y	2449	A
23	Y	2462	G
23	Y	2463	G
23	Y	2490	A
23	Y	2503	G
23	Y	2507	C
23	Y	2511	A
23	Y	2521	C
23	Y	2529	A
23	Y	2530	C
23	Y	2532	G
23	Y	2543	U
23	Y	2544	U
23	Y	2545	G
23	Y	2548	U
23	Y	2558	C
23	Y	2559	A
23	Y	2571	C
23	Y	2574	C
23	Y	2581	G
23	Y	2607	G
23	Y	2609	A
23	Y	2627	C
23	Y	2630	A
23	Y	2646	C
23	Y	2647	U
23	Y	2649	A
23	Y	2652	G
23	Y	2653	G
23	Y	2654	A
23	Y	2655	U
23	Y	2665	C

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Mol	Chain	Res	Type
23	Y	2671	G
23	Y	2672	A
23	Y	2694	G
23	Y	2698	C
23	Y	2699	C
23	Y	2700	A
23	Y	2702	A
23	Y	2705	G
23	Y	2713	G
23	Y	2715	U
23	Y	2722	C
23	Y	2726	G
23	Y	2727	A
23	Y	2728	U
23	Y	2729	G
23	Y	2737	G
23	Y	2742	A
23	Y	2744	C
23	Y	2753	G
23	Y	2790	A
23	Y	2791	G
23	Y	2796	A
23	Y	2806	G
23	Y	2809	U
23	Y	2821	G
23	Y	2823	G
23	Y	2826	A
23	Y	2833	U
23	Y	2837	U
23	Y	2853	C
23	Y	2871	U
23	Y	2913	U
23	Y	2914	A
23	Y	2915	C
23	Y	2926	A
23	Y	2936	C
23	Y	2938	G
23	Y	2953	U
23	Y	2957	A
23	Y	2972	A
23	Y	2974	A
23	Y	2976	C

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Mol	Chain	Res	Type
23	Y	2981	A
23	Y	2982	A
23	Y	2985	G
23	Y	2986	G
23	Y	3002	A
23	Y	3009	U
23	Y	3013	C
23	Y	3014	A
23	Y	3015	C
23	Y	3021	A
23	Y	3022	G
23	Y	3042	A
23	Y	3070	G
23	Y	3088	C
23	Y	3093	A
23	Y	3101	C
23	Y	3105	C
23	Y	3106	C
23	Y	3107	G
23	Y	3108	G
23	Y	3112	A
23	Y	3114	A
23	Y	3115	A
24	U	4	A
24	U	9	G
24	U	11	U
24	U	12	C
24	U	13	C
24	U	42	C
24	U	43	C
24	U	52	G
24	U	67	A
24	U	87	U
24	U	89	C
24	U	90	G
24	U	107	A

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	92	A
1	A	194	A

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Mol	Chain	Res	Type
1	A	422	C
1	A	429	U
1	A	485	G
1	A	498	C
1	A	512	A
1	A	895	A
1	A	997	A
1	A	1011	U
1	A	1058	U
1	A	1109	C
1	A	1117	U
1	A	1149	C
1	A	1477	A
1	A	1482	U
23	Y	89	A
23	Y	97	U
23	Y	313	G
23	Y	316	U
23	Y	322	A
23	Y	335	G
23	Y	336	C
23	Y	357	U
23	Y	445	U
23	Y	452	G
23	Y	974	G
23	Y	980	C
23	Y	981	U
23	Y	1004	C
23	Y	1010	U
23	Y	1046	C
23	Y	1084	U
23	Y	1186	G
23	Y	1231	U
23	Y	1436	C
23	Y	1473	G
23	Y	1532	G
23	Y	1634	C
23	Y	1636	A
23	Y	1730	U
23	Y	2074	G
23	Y	2088	C
23	Y	2094	G

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Mol	Chain	Res	Type
23	Y	2166	C
23	Y	2236	G
23	Y	2282	A
23	Y	2580	G
23	Y	2693	A
23	Y	3008	C
24	U	10	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 629 ligands modelled in this entry, 629 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	Y	31

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Mol	Chain	Number of breaks
30	e	20
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	2406:U	O3'	2407:C	P	20.82
1	Y	1008:G	O3'	1009:U	P	11.65
1	e	22:PRO	C	23:ALA	N	10.56
1	Y	2096:G	O3'	2097:G	P	8.31
1	e	15:ILE	C	16:GLN	N	8.16
1	Y	996:G	O3'	997:G	P	7.88
1	Y	1001:C	O3'	1002:C	P	7.49
1	e	118:LEU	C	119:ASN	N	7.48
1	e	54:ASN	C	55:VAL	N	7.41
1	e	42:LYS	C	43:ALA	N	6.99
1	e	25:PRO	C	26:VAL	N	6.54
1	Y	2411:U	O3'	2412:U	P	6.48
1	Y	999:C	O3'	1000:C	P	5.54
1	e	125:ALA	C	126:ALA	N	5.34
1	Y	995:U	O3'	996:G	P	5.28
1	e	41:CYS	C	42:LYS	N	5.08
1	e	124:ASP	C	125:ALA	N	5.04
1	Y	2143:A	O3'	2144:C	P	4.99
1	e	39:GLU	C	40:PHE	N	4.96
1	e	88:GLN	C	89:LYS	N	4.69
1	e	24:PRO	C	25:PRO	N	4.64
1	Y	1005:A	O3'	1006:G	P	4.63
1	Y	367:U	O3'	368:U	P	4.50
1	e	61:THR	C	62:VAL	N	4.47
1	Y	2142:A	O3'	2143:A	P	4.39
1	Y	1196:C	O3'	1197:C	P	4.33
1	Y	2135:U	O3'	2136:A	P	4.23
1	Y	2140:A	O3'	2141:U	P	4.09
1	Y	1170:C	O3'	1171:C	P	4.01
1	Y	279:U	O3'	280:G	P	3.97
1	Y	1210:C	O3'	1211:G	P	3.94
1	e	67:SER	C	68:PHE	N	3.83
1	Y	1631:A	O3'	1632:G	P	3.72
1	e	86:GLY	C	87:VAL	N	3.54
1	Y	2146:A	O3'	2147:U	P	3.53
1	e	55:VAL	C	56:ILE	N	3.45
1	Y	437:G	O3'	438:U	P	3.21

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	13:LEU	C	14:GLN	N	3.19
1	e	68:PHE	C	69:THR	N	3.18
1	Y	454:U	O3'	455:C	P	3.10
1	Y	2087:C	O3'	2088:C	P	3.08
1	e	63:TYR	C	64:GLU	N	3.08
1	e	121:ASN	C	122:ASP	N	3.02
1	Y	1000:C	O3'	1001:C	P	3.01
1	Y	1016:C	O3'	1017:G	P	2.99
1	Y	1019:C	O3'	1020:A	P	2.99
1	Y	1534:C	O3'	1535:C	P	2.99
1	Y	1529:U	O3'	1530:G	P	2.97
1	A	1130:C	O3'	1131:G	P	2.91
1	Y	988:U	O3'	989:G	P	2.89
1	Y	2415:G	O3'	2416:C	P	2.87
1	Y	1708:A	O3'	1709:U	P	2.86

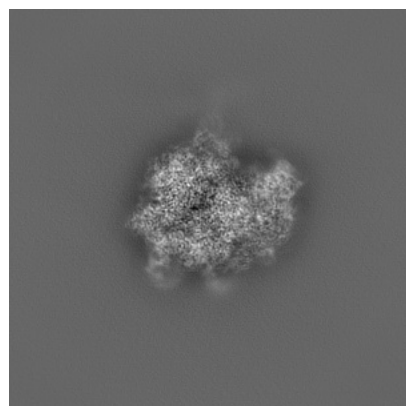
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44091. These allow visual inspection of the internal detail of the map and identification of artifacts.

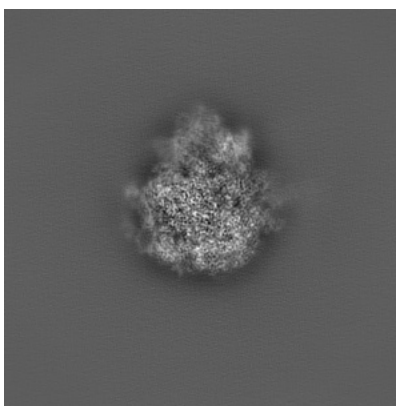
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

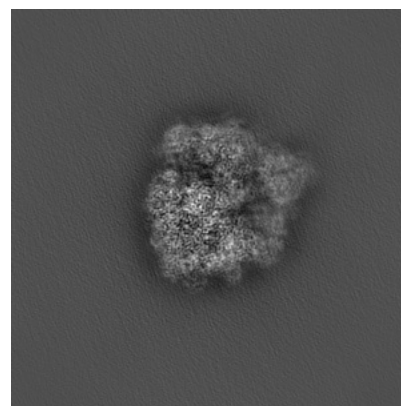
6.1.1 Primary map



X

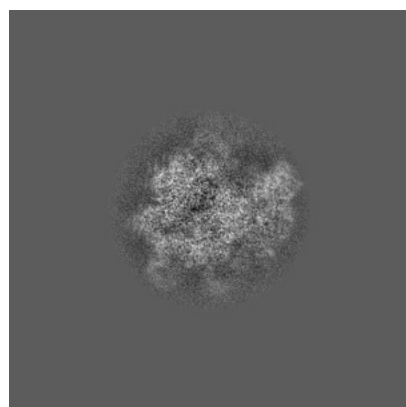


Y

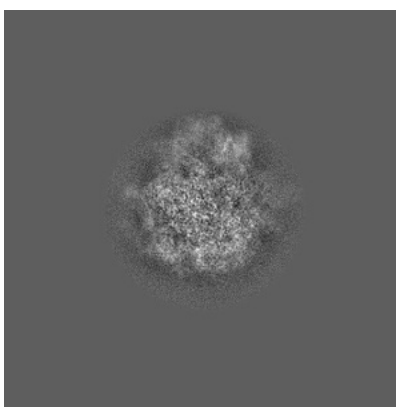


Z

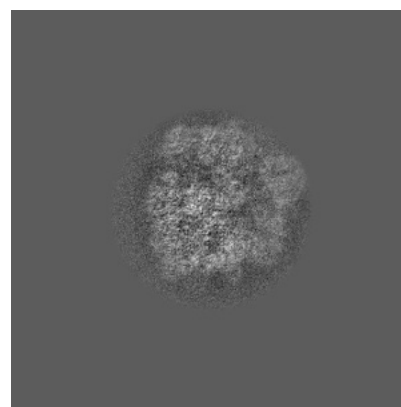
6.1.2 Raw map



X



Y

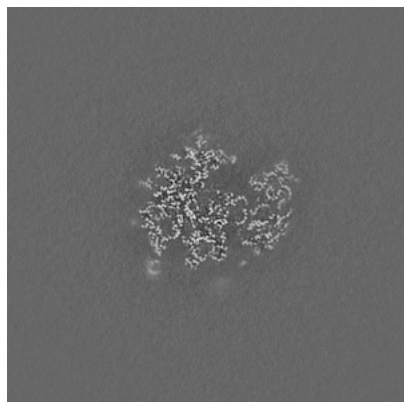


Z

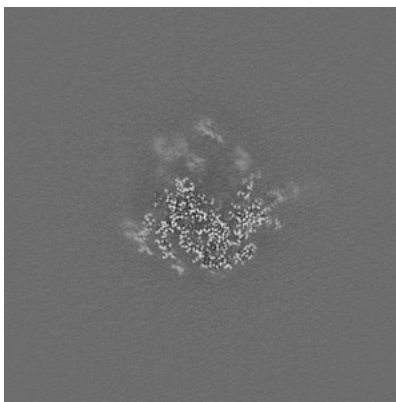
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

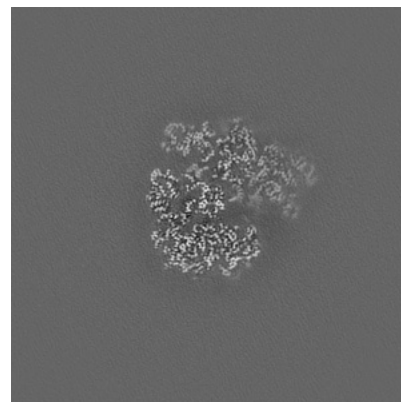
6.2.1 Primary map



X Index: 432

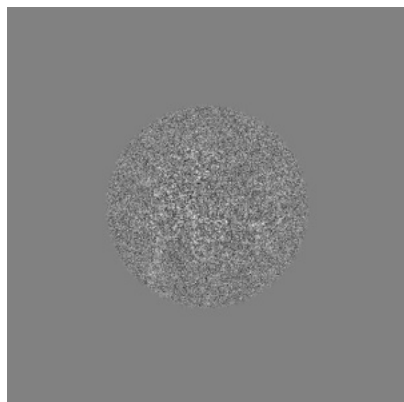


Y Index: 432

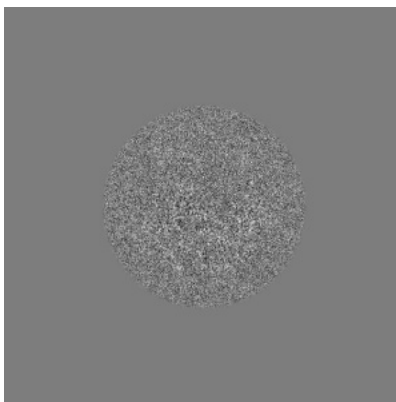


Z Index: 432

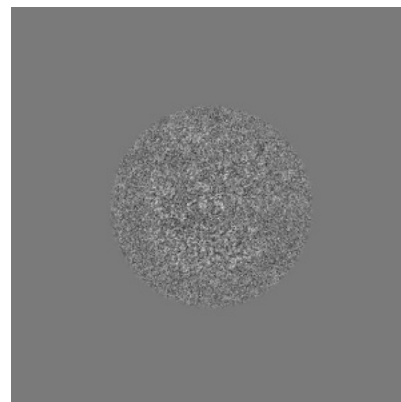
6.2.2 Raw map



X Index: 432



Y Index: 432

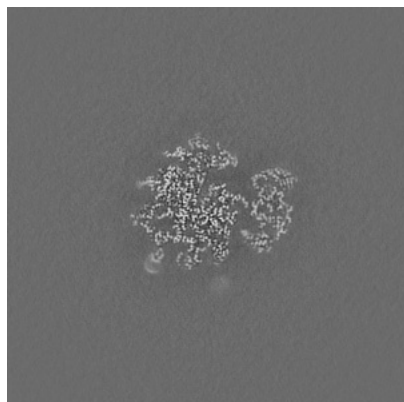


Z Index: 432

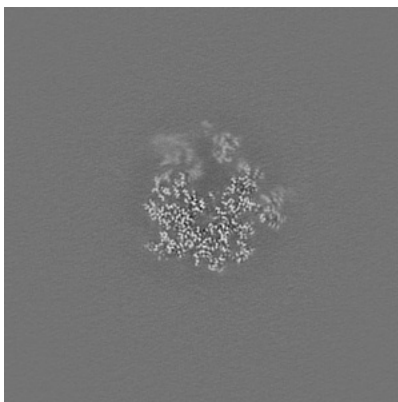
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

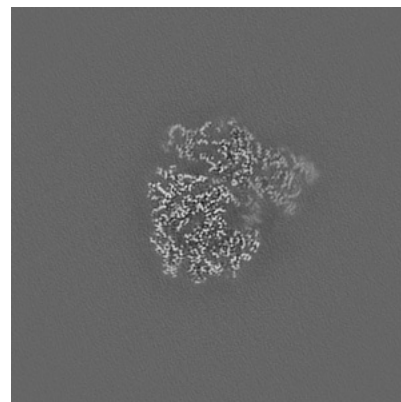
6.3.1 Primary map



X Index: 423

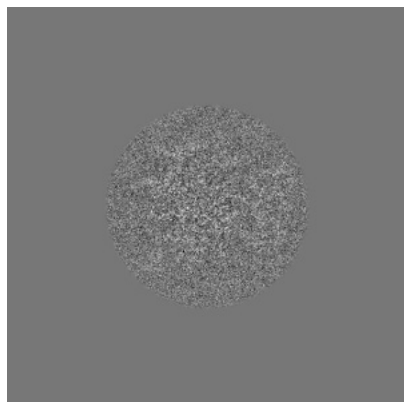


Y Index: 411

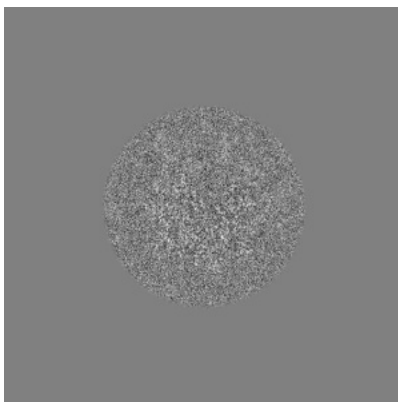


Z Index: 423

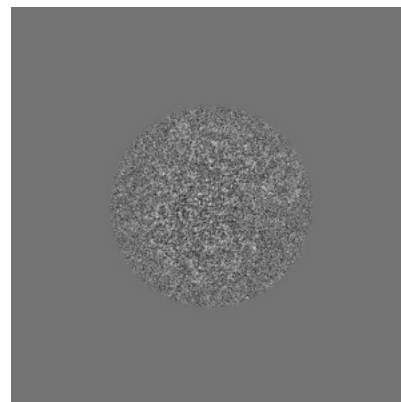
6.3.2 Raw map



X Index: 423



Y Index: 411

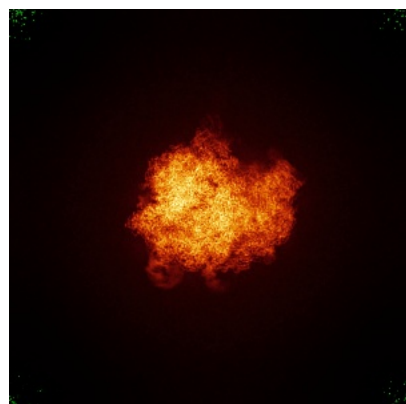


Z Index: 417

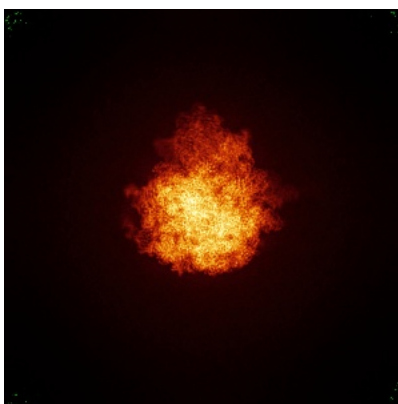
The images above show the largest variance slices of the map in three orthogonal directions.

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

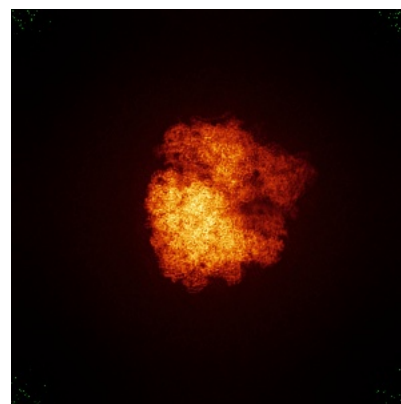
6.4.1 Primary map



X

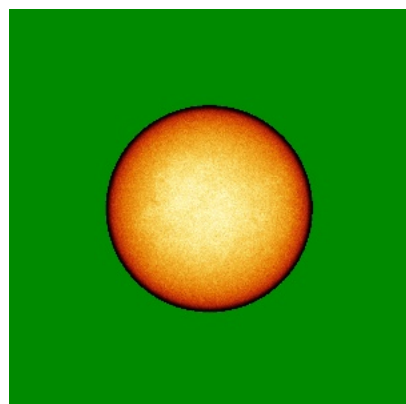


Y

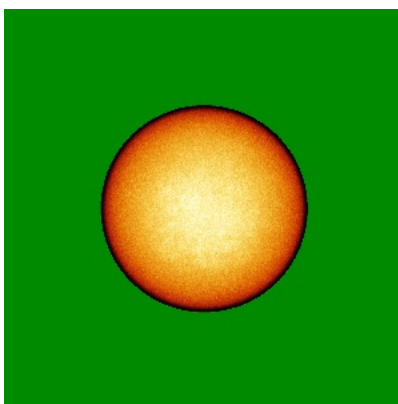


Z

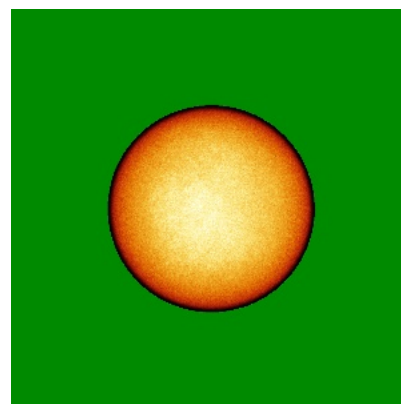
6.4.2 Raw map



X



Y

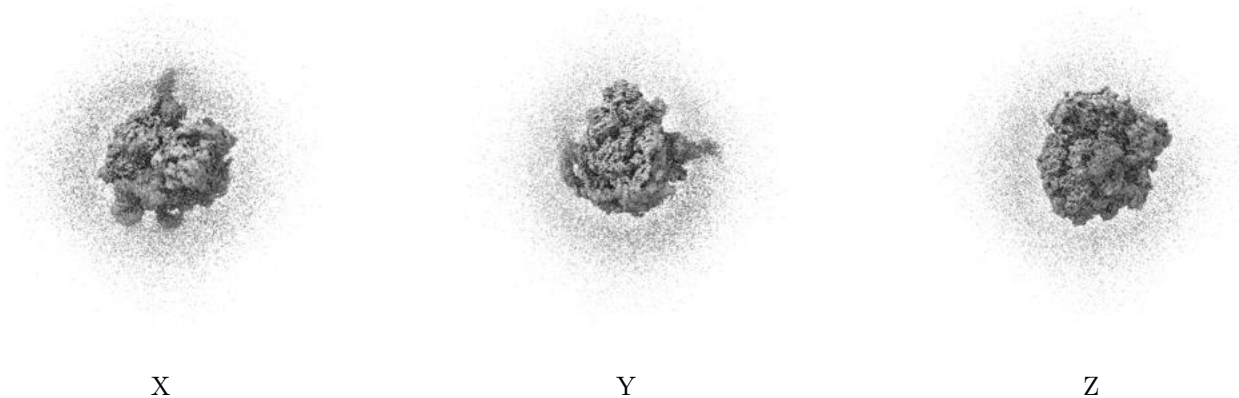


Z

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.

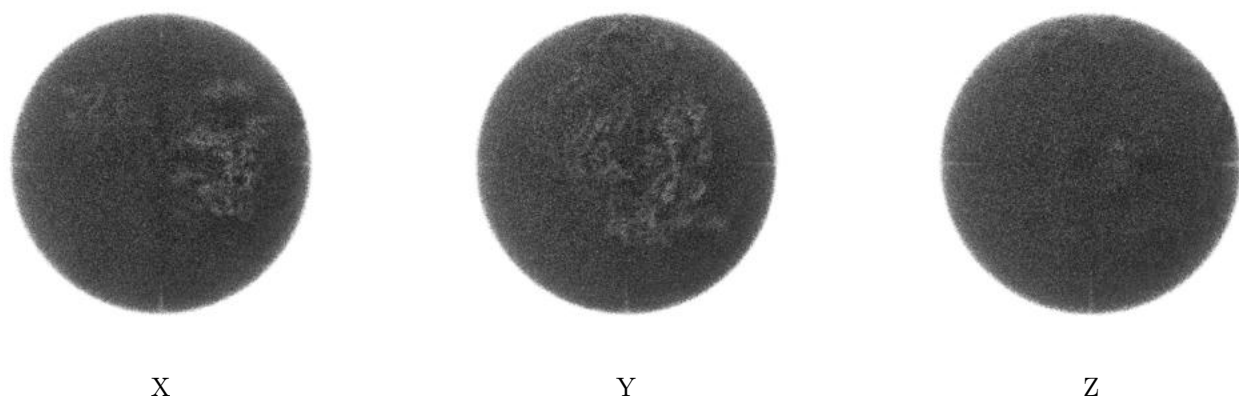
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.901. 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.

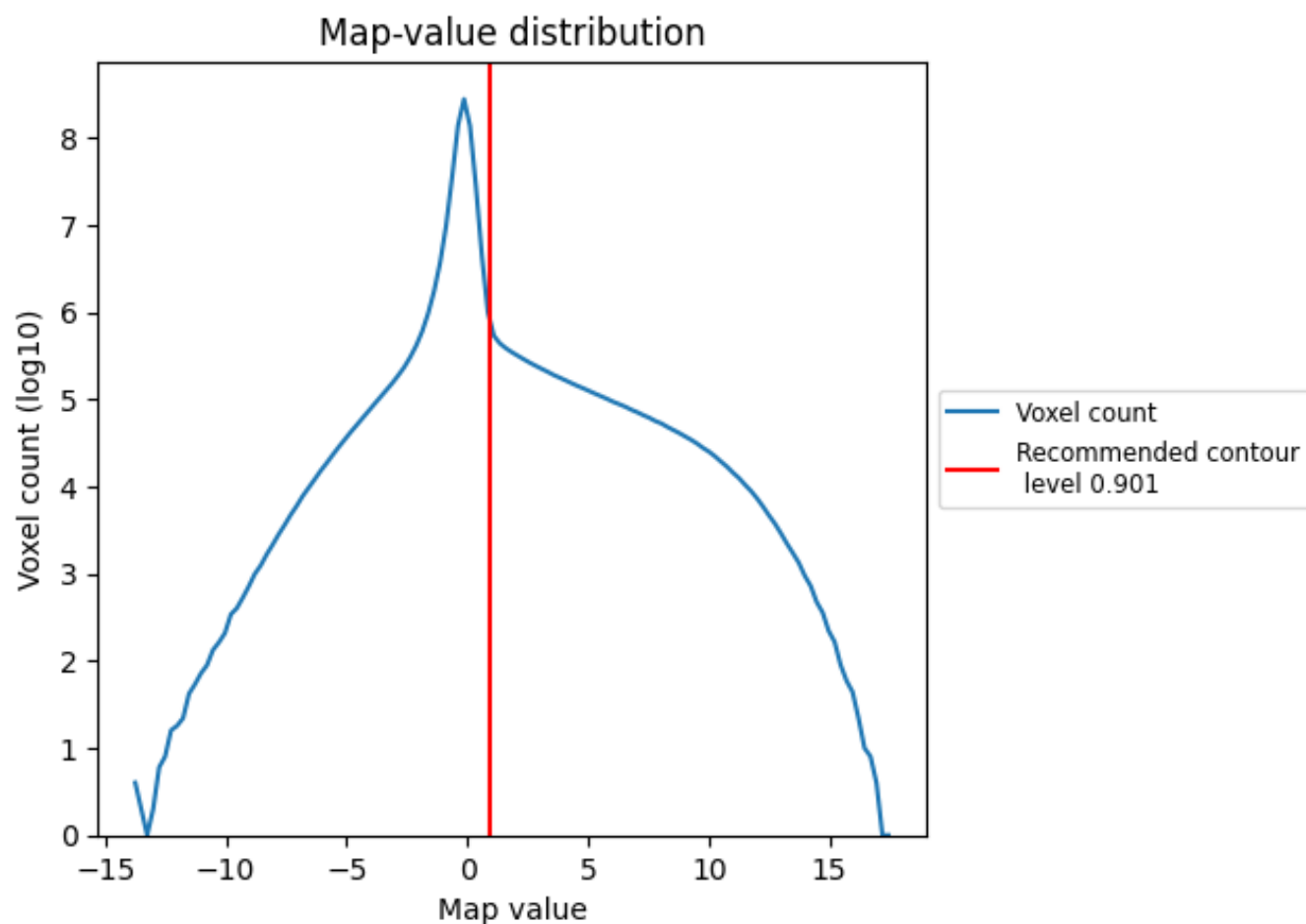
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

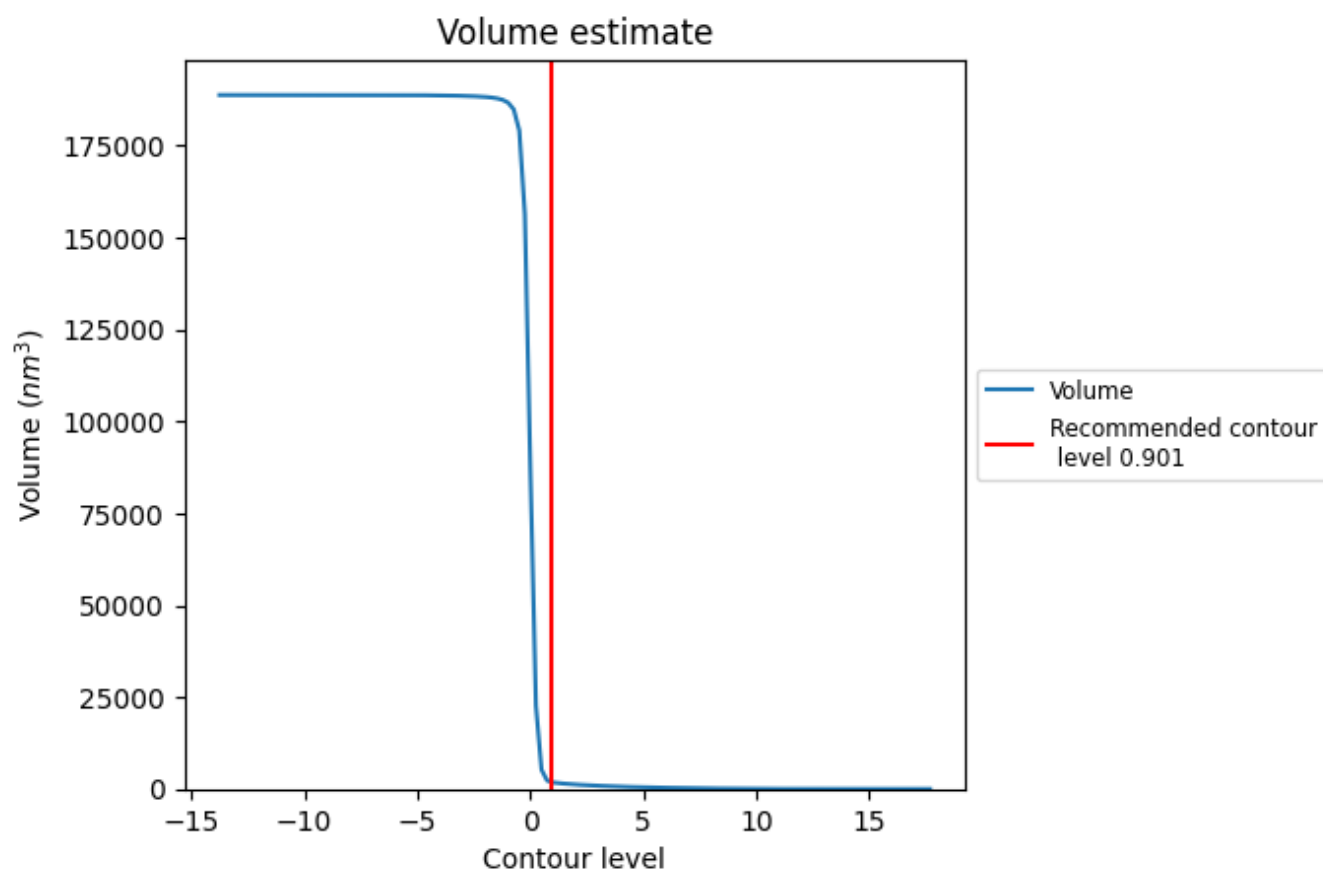
This section contains the results of statistical analysis of the map.

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.

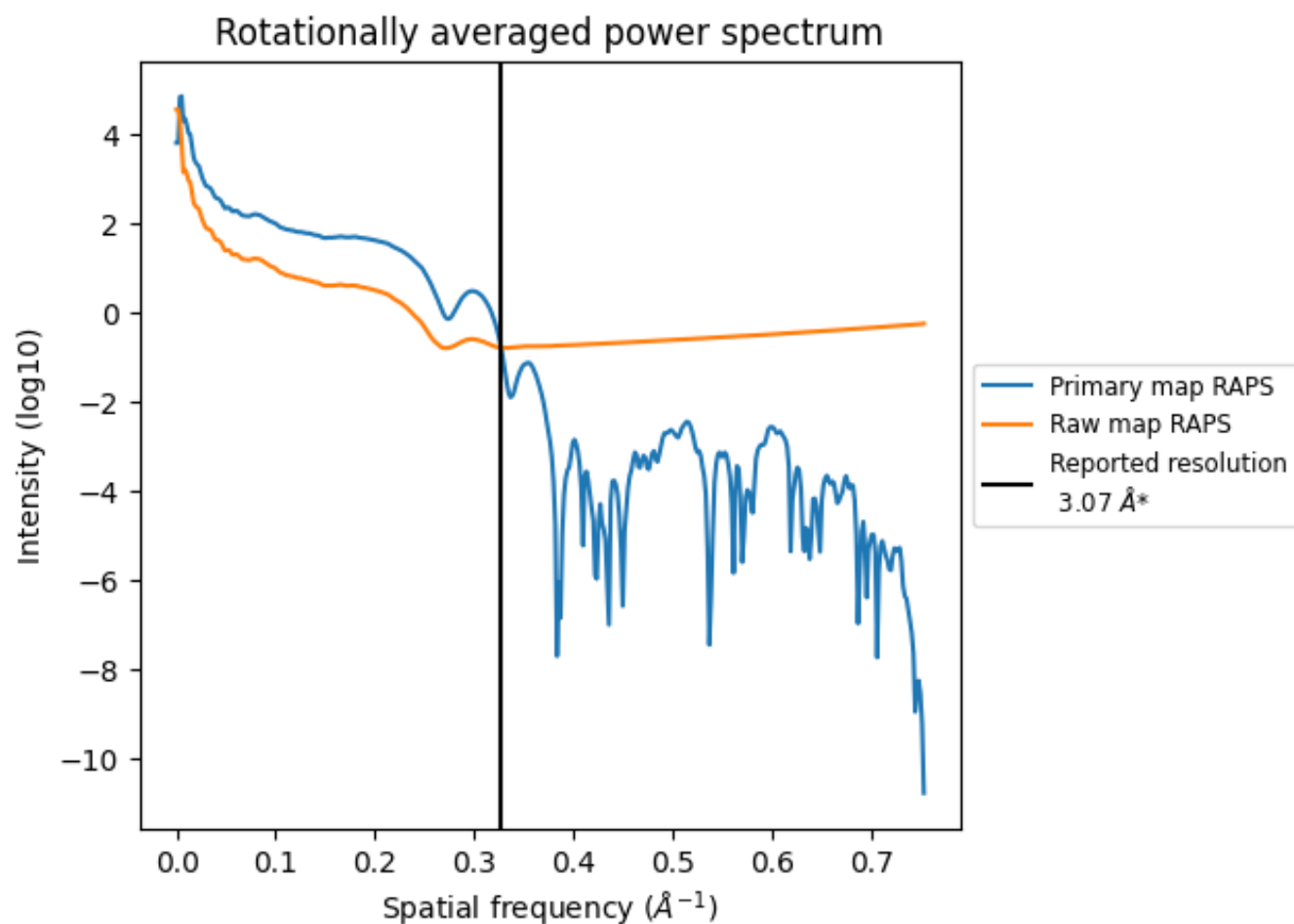
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1958 nm^3 ; this corresponds to an approximate mass of 1768 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 ⓘ

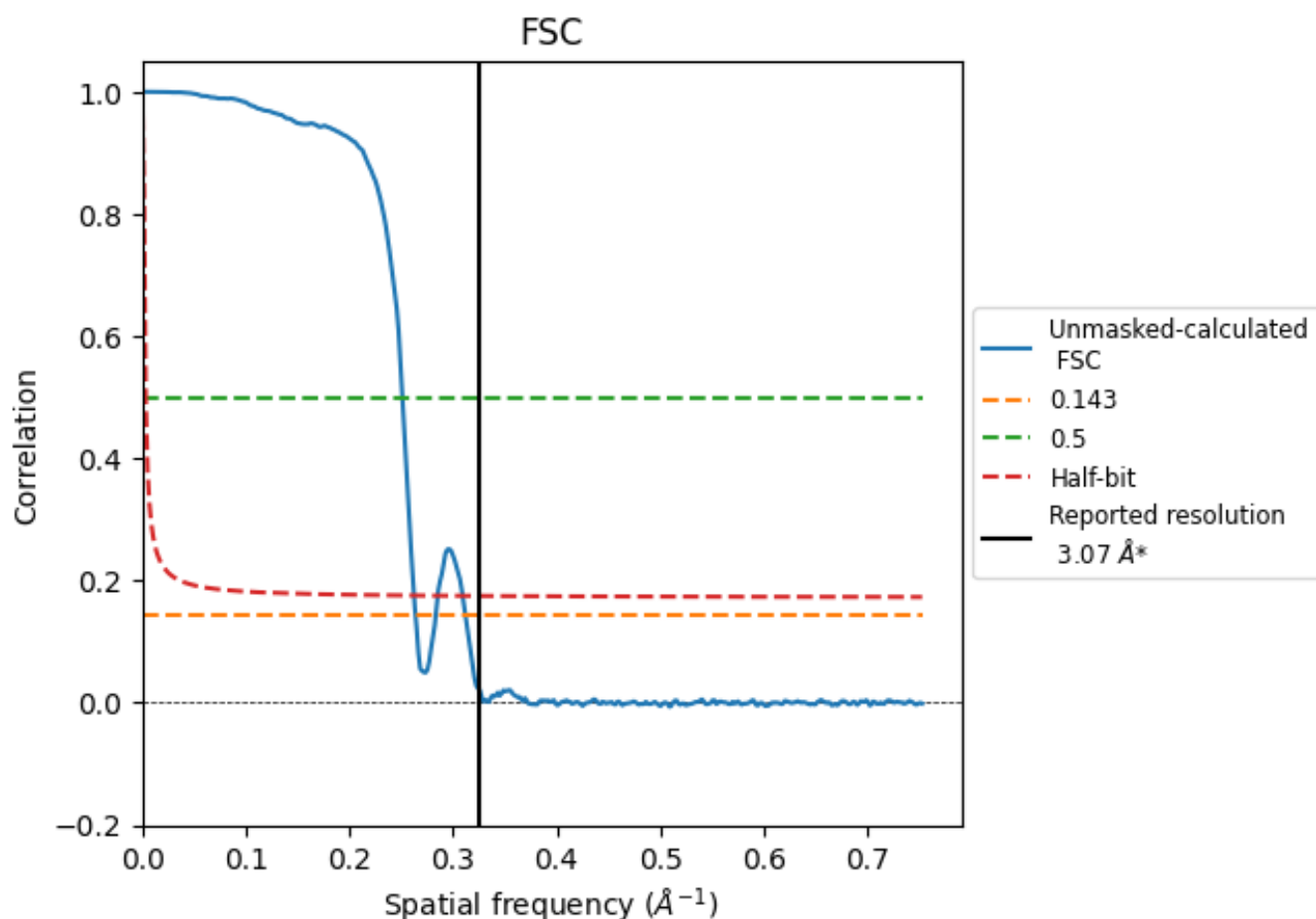


*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.326 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

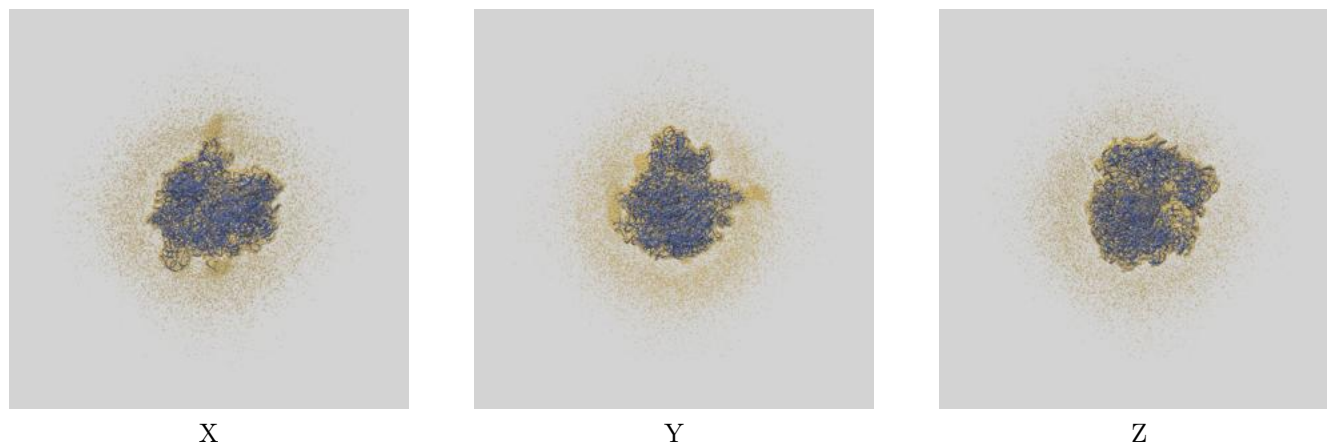
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.79	3.98	3.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 3.07 by more than 10 %

9 Map-model fit [i](#)

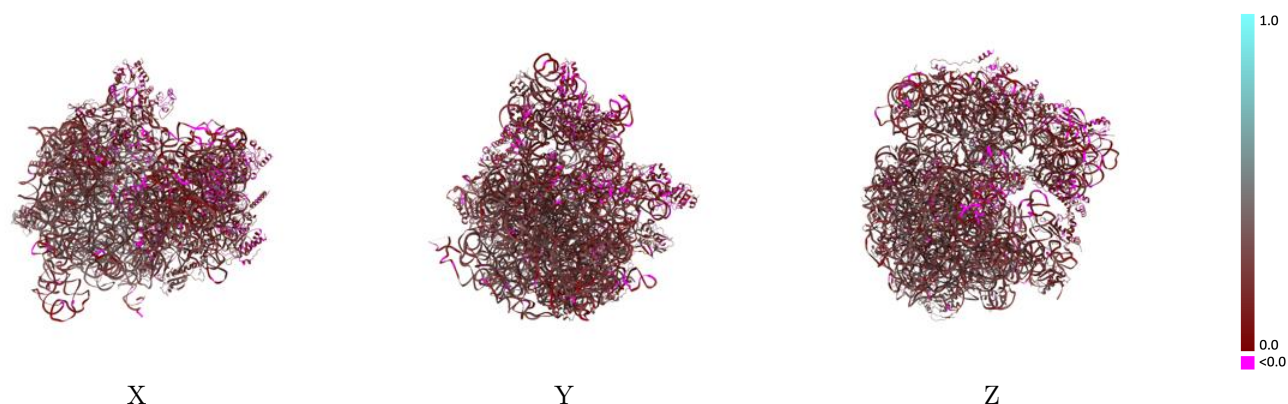
This section contains information regarding the fit between EMDB map EMD-44091 and PDB model 9B1X. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



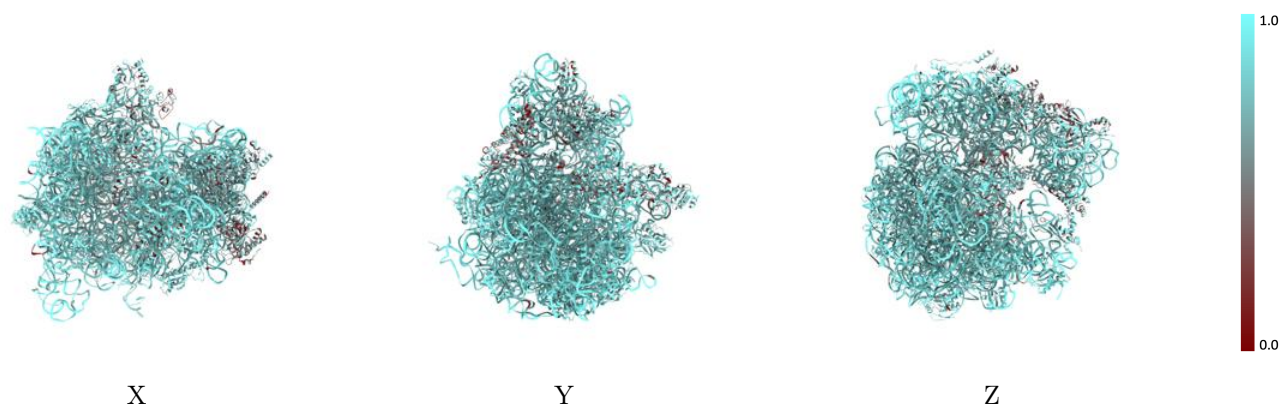
The images above show the 3D surface view of the map at the recommended contour level 0.901 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



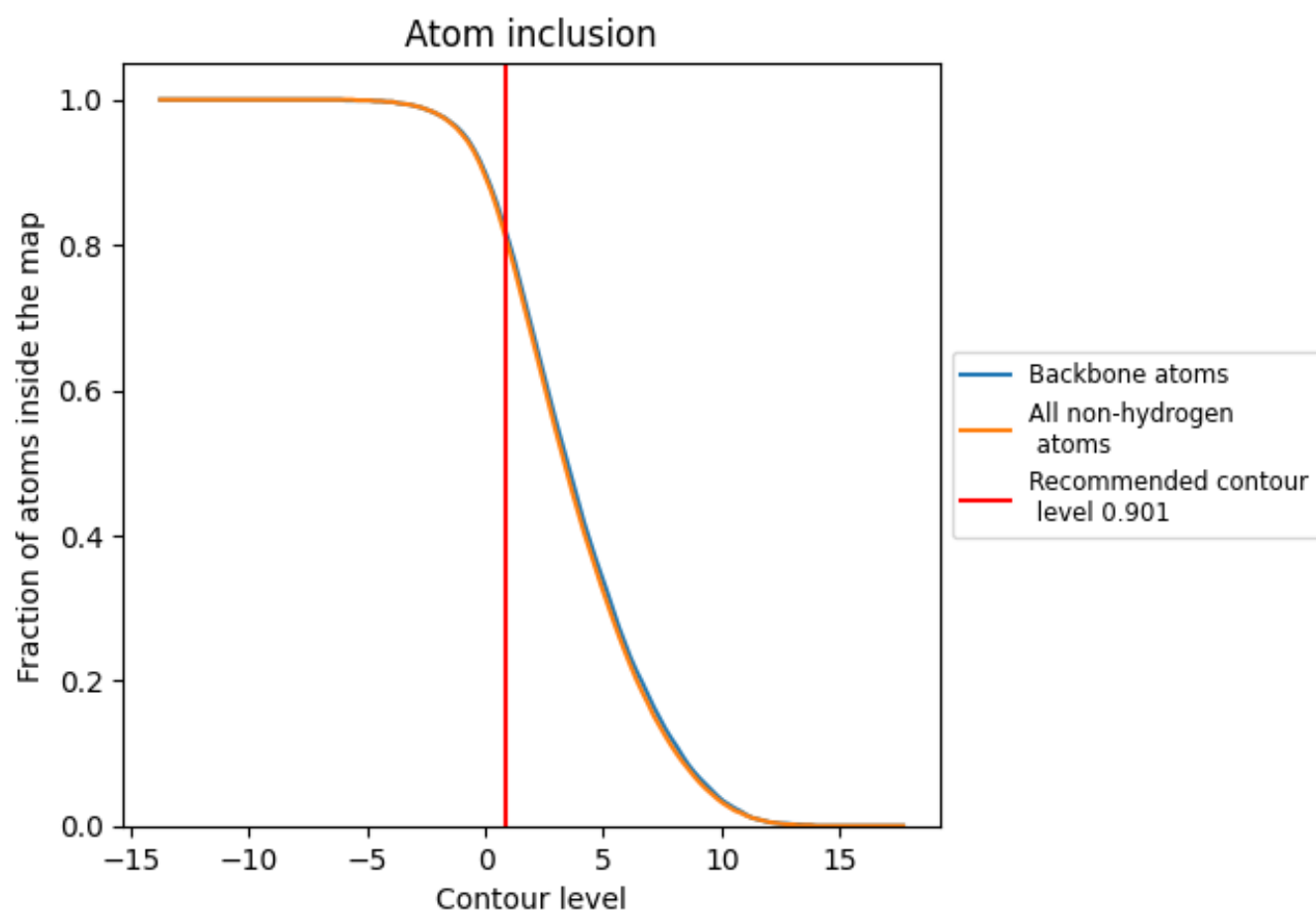
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.901).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.901) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.2300
1	 0.7880	 0.2900
2	 0.7880	 0.2410
5	 0.6760	 0.2300
A	 0.8410	 0.2020
B	 0.6050	 0.2400
C	 0.5710	 0.1140
D	 0.6330	 0.0950
E	 0.6760	 0.1800
F	 0.7990	 0.2600
G	 0.6580	 0.1710
H	 0.7940	 0.2530
I	 0.7970	 0.2440
J	 0.6050	 0.0900
K	 0.7800	 0.2610
L	 0.7280	 0.2450
M	 0.5820	 0.0750
N	 0.6960	 0.1540
O	 0.8020	 0.2690
P	 0.7610	 0.1910
Q	 0.7850	 0.2290
R	 0.8170	 0.2470
S	 0.7360	 0.1100
T	 0.7890	 0.2060
U	 0.8890	 0.2330
V	 0.4030	 0.1560
X	 0.6840	 0.2000
Y	 0.8500	 0.2540
Z	 0.7510	 0.2600
a	 0.7700	 0.2400
b	 0.8270	 0.3020
c	 0.7520	 0.1560
d	 0.8080	 0.2250
e	 0.5670	 0.0880
f	 0.8080	 0.2670



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Chain	Atom inclusion	Q-score
g	 0.7180	 0.2320
h	 0.8190	 0.2990
i	 0.7210	 0.2210
j	 0.8050	 0.2760
k	 0.8450	 0.2490
l	 0.7650	 0.2340
m	 0.8000	 0.2610
n	 0.8270	 0.2630
o	 0.7960	 0.2770
p	 0.8210	 0.2950
q	 0.8380	 0.2810
r	 0.7350	 0.2010
s	 0.7760	 0.2690
t	 0.7650	 0.2790
u	 0.8100	 0.2710
v	 0.7060	 0.1030
w	 0.7910	 0.2690
x	 0.8280	 0.3010
y	 0.7950	 0.2410
z	 0.8110	 0.3220