Full wwPDB EM Validation Report

May 18, 2025 – 04:15 AM EDT

PDB ID	:	9BSS / pdb_00009bss
EMDB ID	:	EMD-44871
Title	:	45SRbgA particle in complex with RbgA and YphC. Class B
Authors	:	Arpin, D.; Ortega, J.
Deposited on	:	2024-05-13
Resolution	:	3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

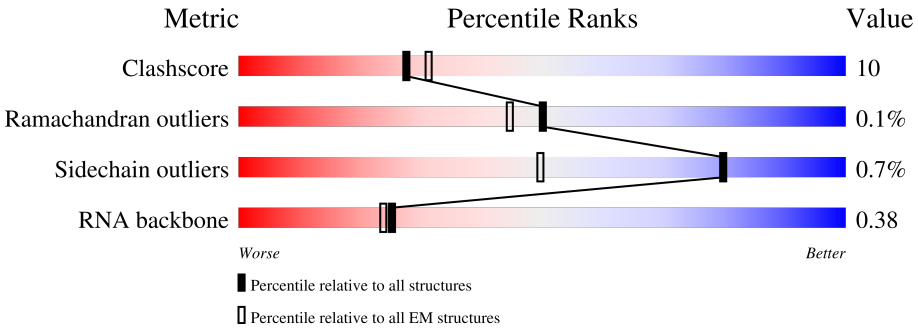
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=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	2927	7% 45% 28% 15% 12%
2	B	119	58% 13% 48% 34% 6%
3	C	277	81% 8% 11%
4	D	209	90% 9%
5	E	207	7% 92% 7%
6	F	179	89% 66% 31%
7	G	145	97%

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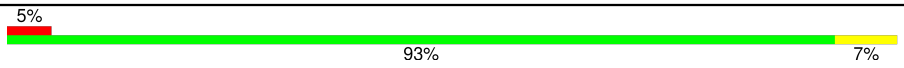
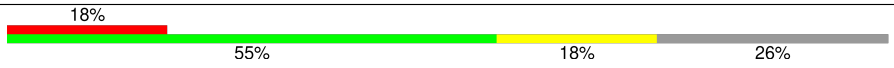
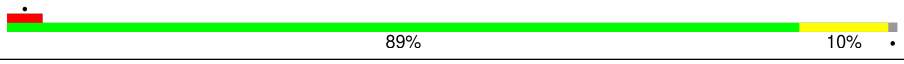
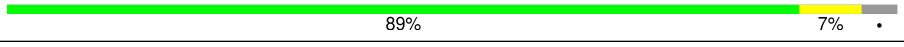
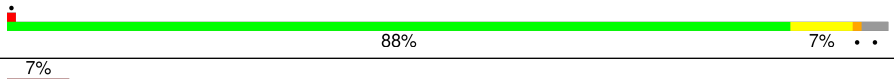
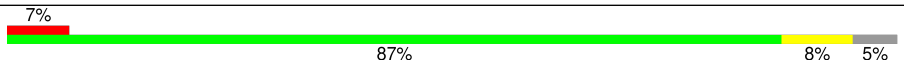
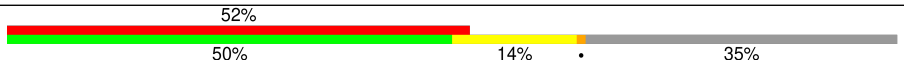
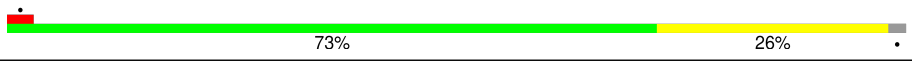
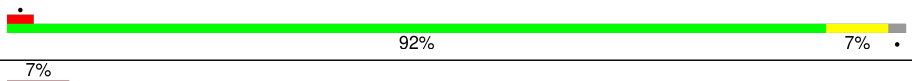
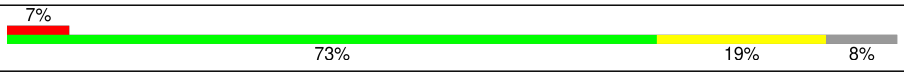
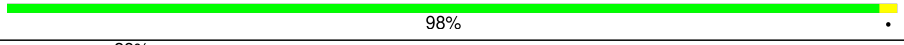
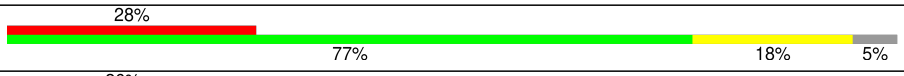
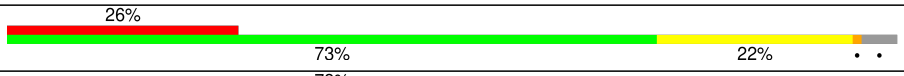
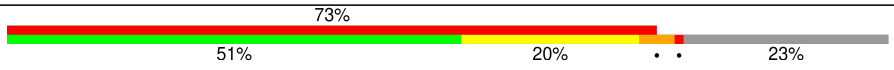
Mol	Chain	Length	Quality of chain
8	H	122	
9	I	146	
10	J	120	
11	K	115	
12	L	118	
13	M	102	
14	N	113	
15	O	95	
16	P	103	
17	Q	94	
18	R	66	
19	S	59	
20	T	59	
21	U	44	
22	V	282	
23	W	436	
24	Y	232	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 81609 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2572	55237	24642	10204	17819	2572	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1558	C	G	conflict	GB 467326

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	112	2395	1068	435	780	112	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	246	1895	1177	373	340	5	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	207	1575	988	290	292	5	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	205	1551	974	288	287	2	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	175	Total	C	N	O	S	0	0
			1285	793	237	254	1		

- Molecule 7 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 9 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	108	Total	C	N	O	S	0	0
			753	461	146	145	1		

- Molecule 10 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 11 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	113	Total	C	N	O	0	0
			925	589	180	156		

- Molecule 12 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	117	Total	C	N	O	S	0	0
			934	588	186	156	4		

- Molecule 13 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	101	Total	C	N	O	0	0
			786	501	139	146		

- Molecule 14 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 15 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	92	Total	C	N	O	S	0	0
			741	464	136	138	3		

- Molecule 16 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	98	Total	C	N	O	S	0	0
			737	463	137	133	4		

- Molecule 17 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	61	Total	C	N	O	0	0
			423	261	79	83		

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 19 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 20 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	54	Total	C	N	O	S	0	0
			394	241	80	68	5		

- Molecule 21 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 22 is a protein called Ribosome biogenesis GTPase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	267	Total	C	N	O	S	0	0
			2119	1349	378	387	5		

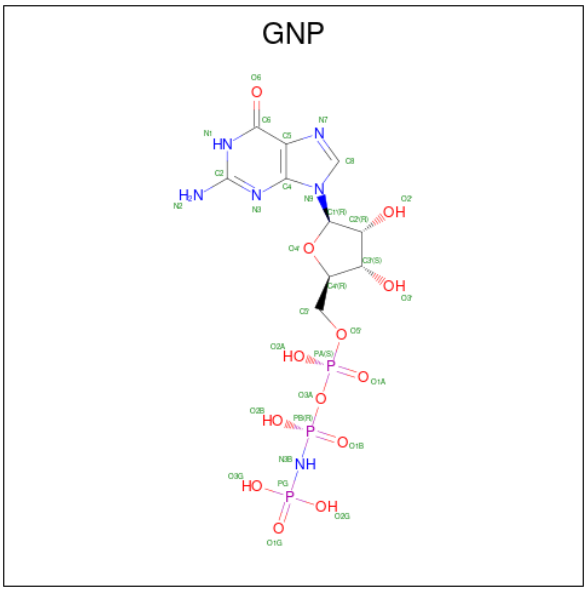
- Molecule 23 is a protein called GTPase Der.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	417	Total	C	N	O	S	0	0
			3239	2056	559	615	9		

- Molecule 24 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	178	Total	C	N	O	S	0	0
			1334	853	223	254	4		

- Molecule 25 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



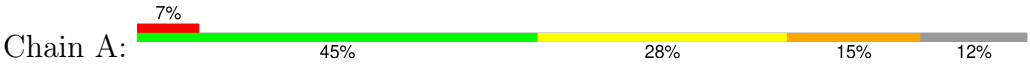
Mol	Chain	Residues	Atoms					AltConf
25	V	1	Total	C	N	O	P	0
			32	10	6	13	3	
25	W	1	Total	C	N	O	P	0
			32	10	6	13	3	
25	W	1	Total	C	N	O	P	0
			32	10	6	13	3	

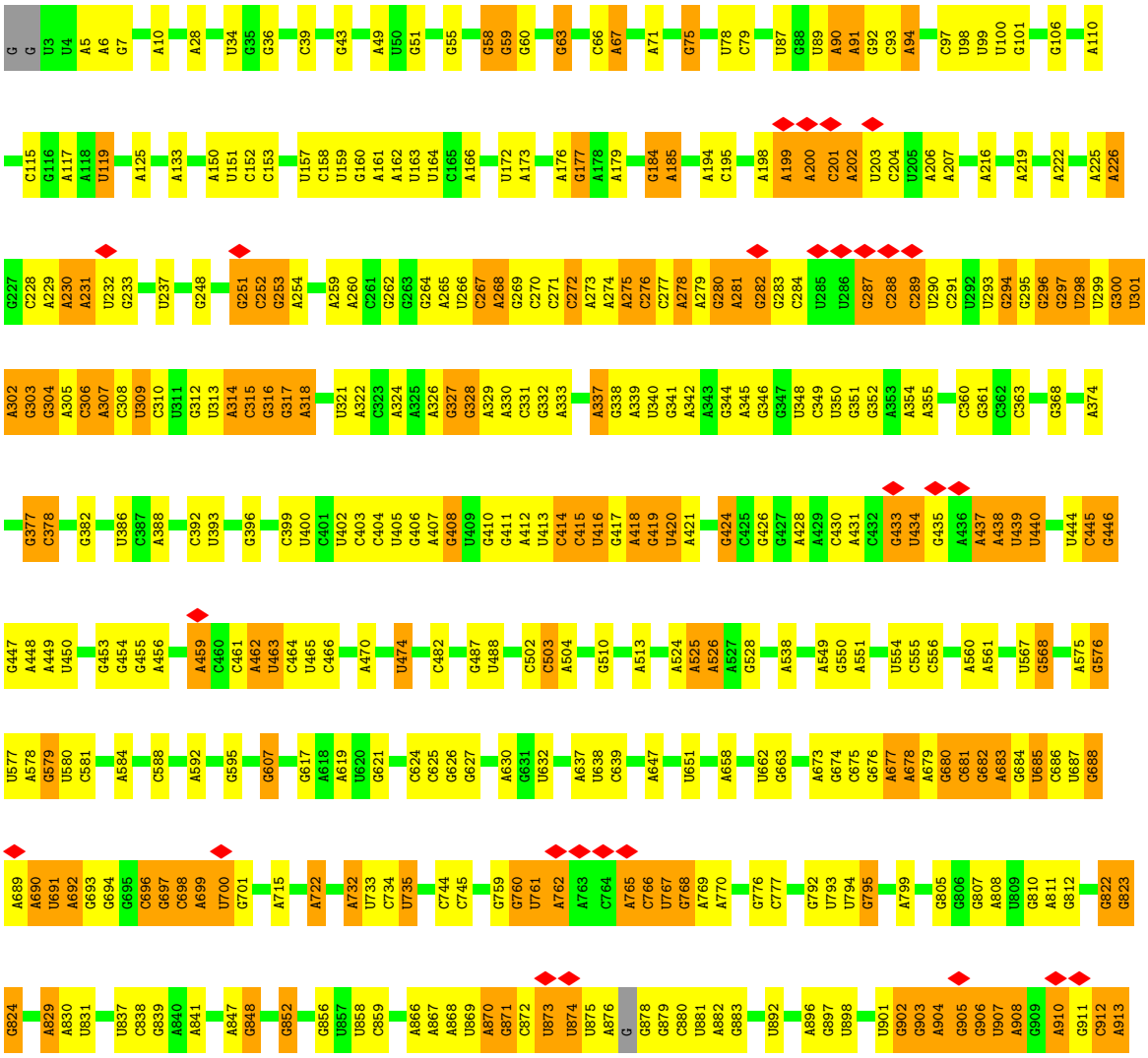
3 Residue-property plots (i)

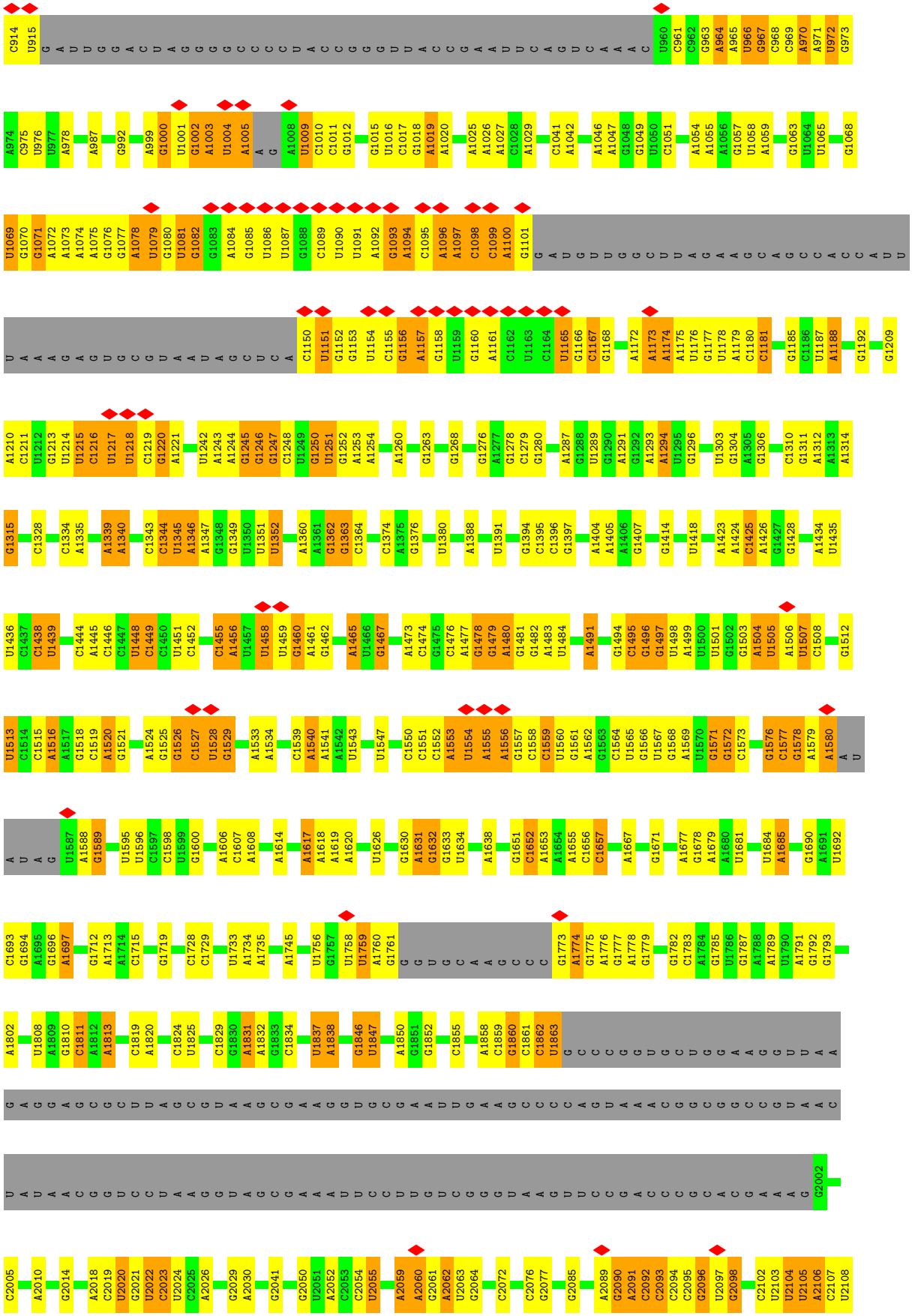
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

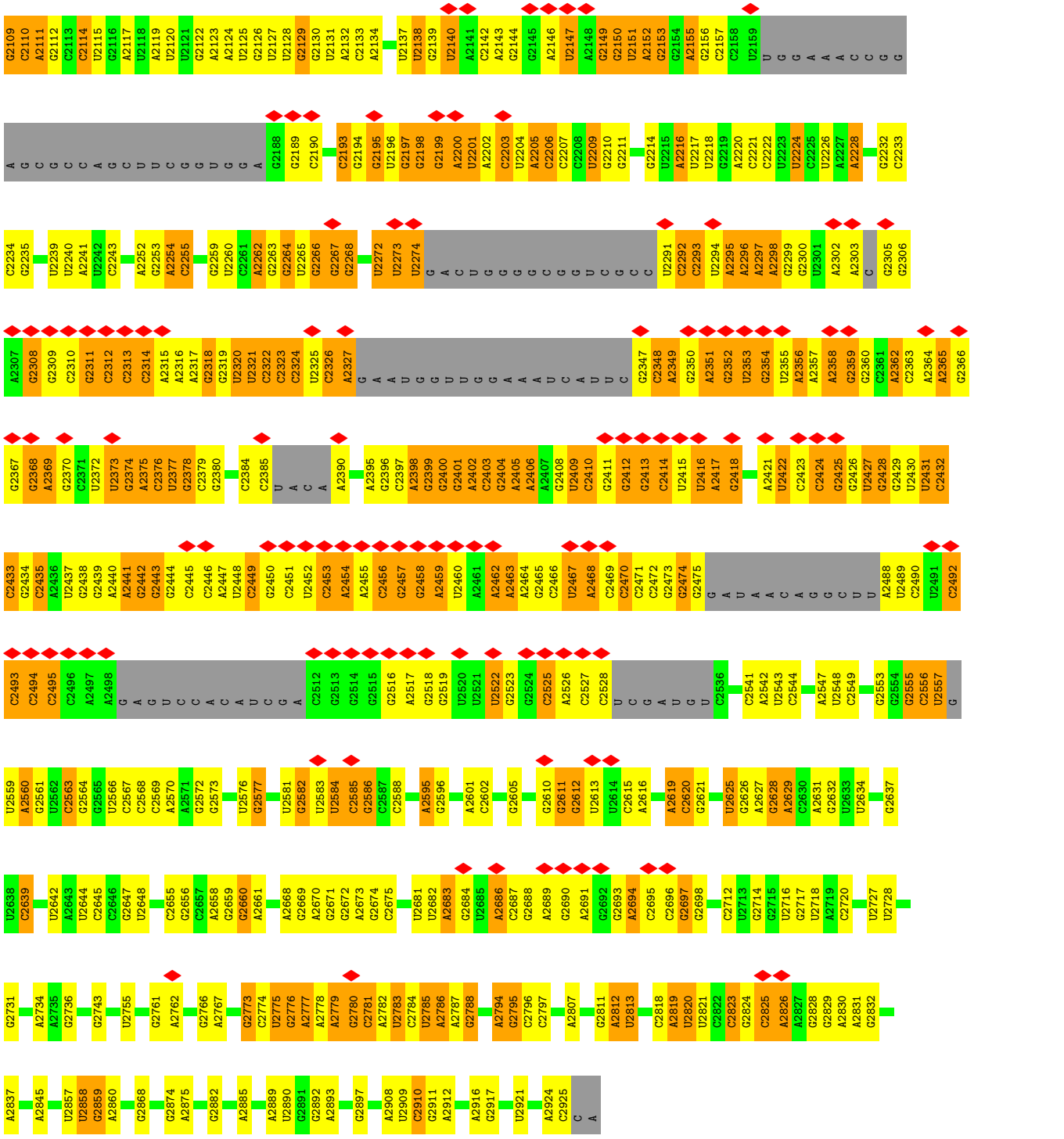
- Molecule 1: 23S rRNA

Chain A:





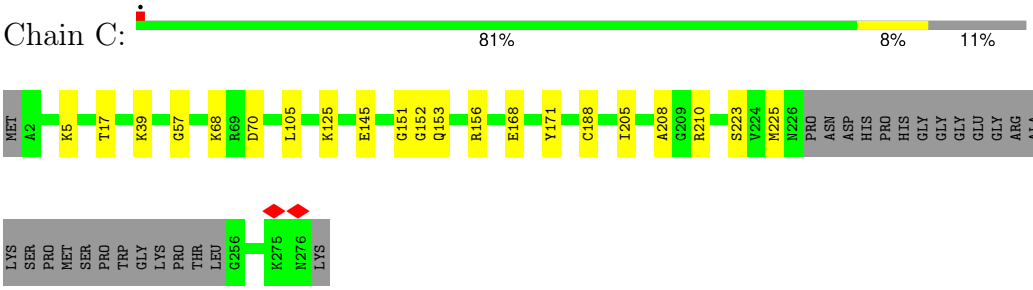




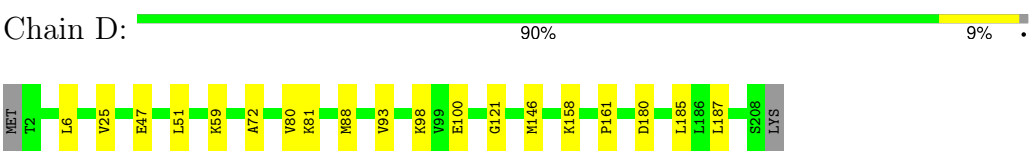
• Molecule 2: 5S rRNA

Chain B:

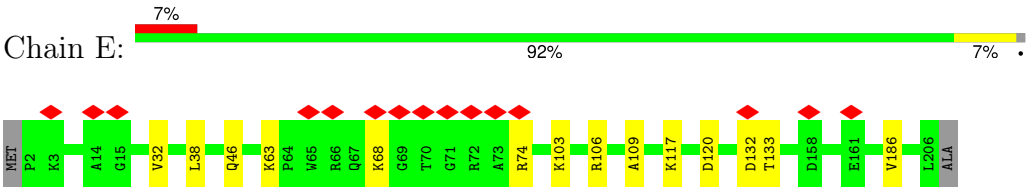
• Molecule 3: Large ribosomal subunit protein uL2



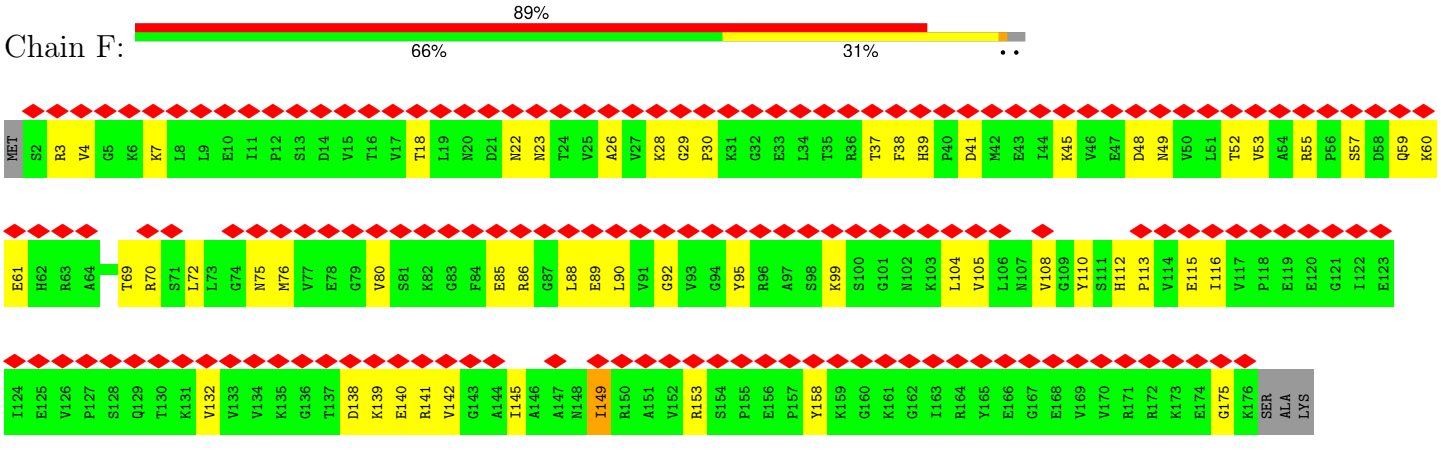
• Molecule 4: Large ribosomal subunit protein uL3



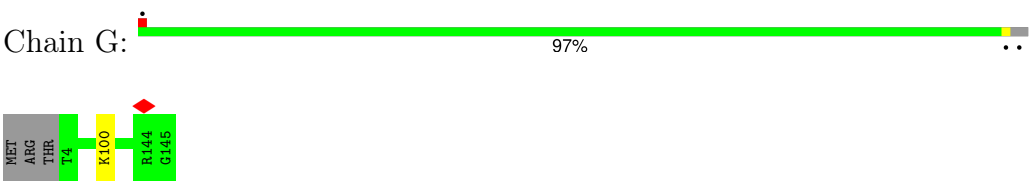
• Molecule 5: Large ribosomal subunit protein uL4



• Molecule 6: Large ribosomal subunit protein uL6

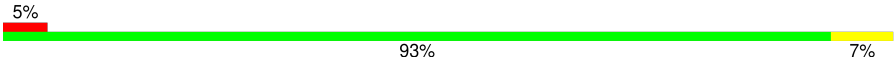


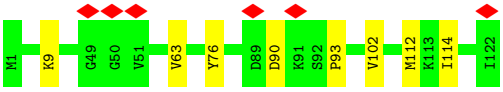
• Molecule 7: Large ribosomal subunit protein uL13



• Molecule 8: Large ribosomal subunit protein uL14

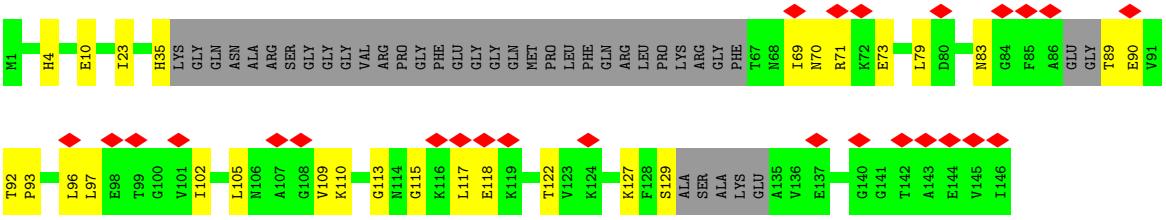
Chain H:





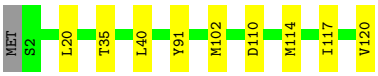
• Molecule 9: Large ribosomal subunit protein uL15

Chain I:



• Molecule 10: Large ribosomal subunit protein bL17

Chain J:



• Molecule 11: Large ribosomal subunit protein bL19

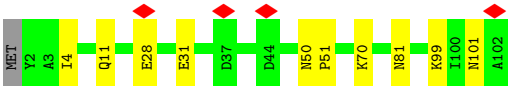
Chain K:

• Molecule 12: Large ribosomal subunit protein bL20

Chain L:

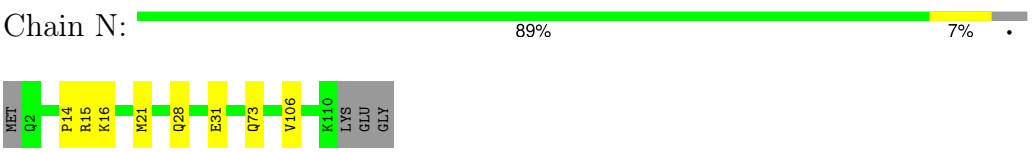
• Molecule 13: Large ribosomal subunit protein bL21

Chain M:



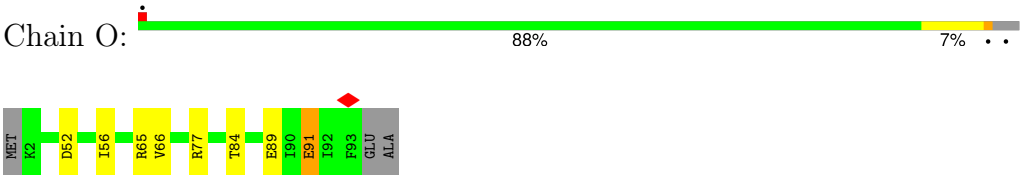
• Molecule 14: Large ribosomal subunit protein uL22

Chain N:



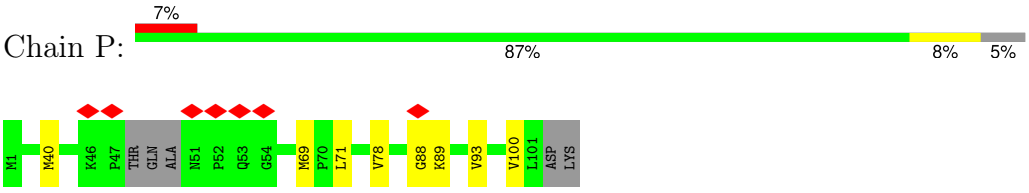
• Molecule 15: Large ribosomal subunit protein uL23

Chain O:



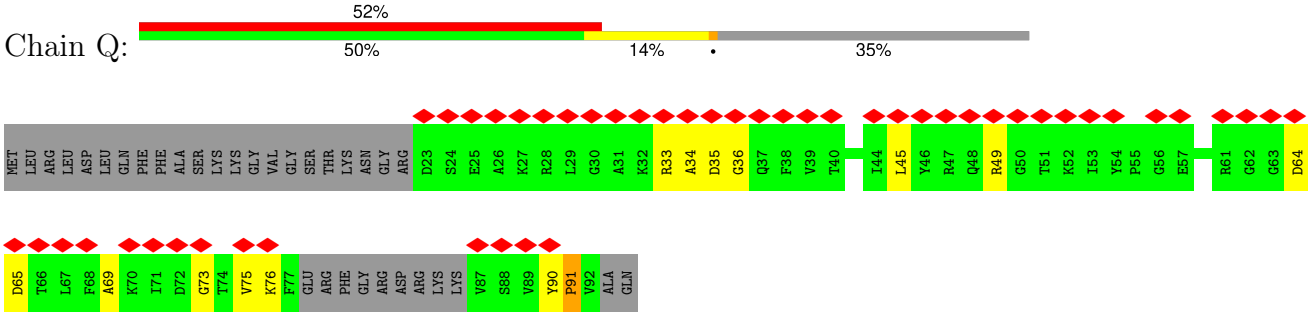
• Molecule 16: Large ribosomal subunit protein uL24

Chain P:



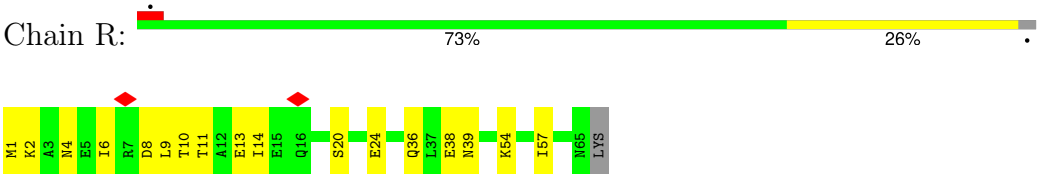
• Molecule 17: Large ribosomal subunit protein bL27

Chain Q:



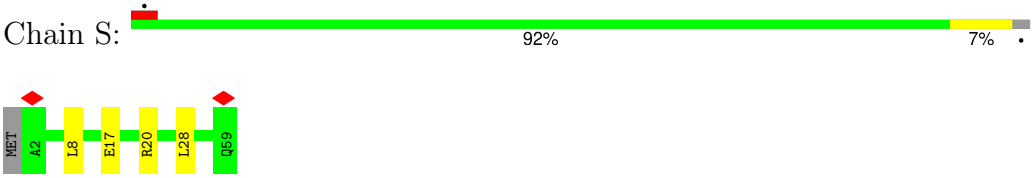
• Molecule 18: Large ribosomal subunit protein uL29

Chain R:



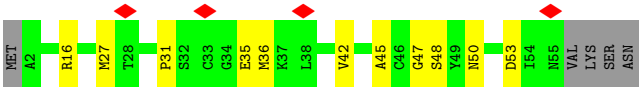
• Molecule 19: Large ribosomal subunit protein uL30

Chain S:



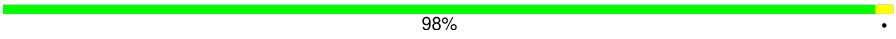
• Molecule 20: Large ribosomal subunit protein bL32

Chain T:



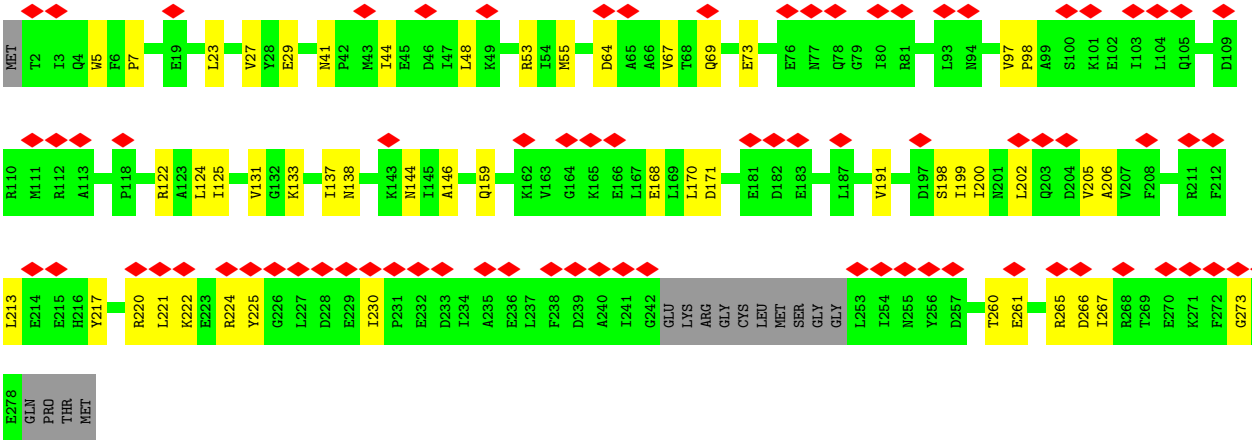
• Molecule 21: Large ribosomal subunit protein bL34

Chain U:



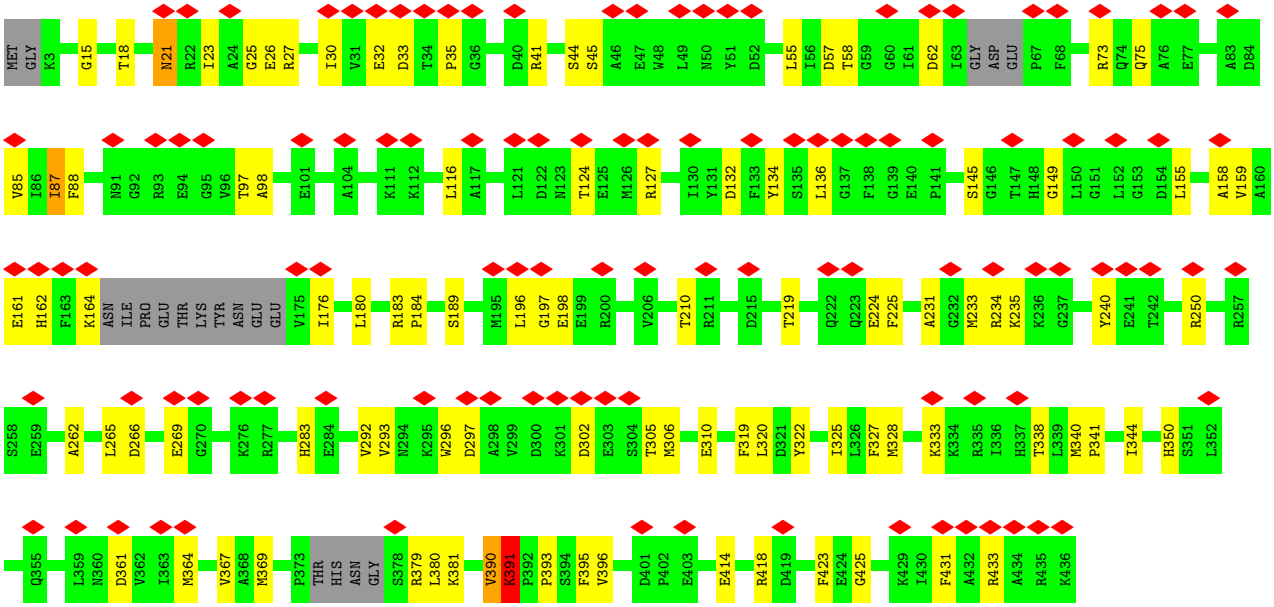
• Molecule 22: Ribosome biogenesis GTPase A

Chain V:



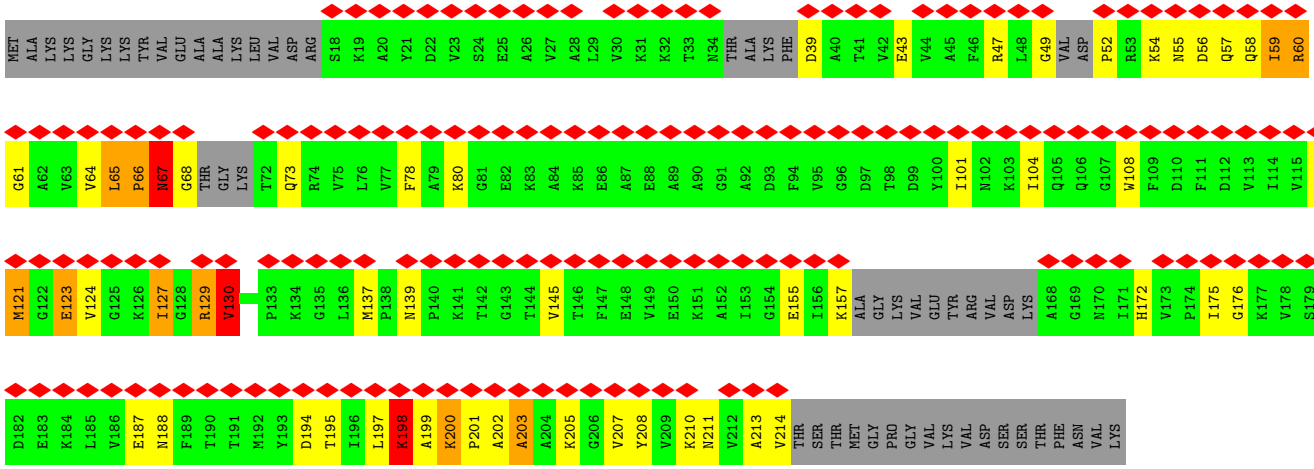
• Molecule 23: GTPase Der

Chain W:



• Molecule 24: Large ribosomal subunit protein uL1

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.607	Depositor
Minimum map value	-0.197	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.146	Depositor
Map size (Å)	383.04, 383.04, 383.04	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/61858	0.32	0/96468
2	B	0.13	0/2678	0.34	0/4174
3	C	0.17	0/1921	0.42	3/2570 (0.1%)
4	D	0.16	0/1597	0.35	0/2140
5	E	0.15	0/1570	0.31	0/2119
6	F	0.16	0/1303	0.46	1/1760 (0.1%)
7	G	0.16	0/1146	0.29	0/1542
8	H	0.16	0/927	0.32	0/1245
9	I	0.18	0/754	0.50	0/1007
10	J	0.17	0/960	0.31	0/1284
11	K	0.15	0/938	0.35	0/1255
12	L	0.20	0/946	0.35	0/1259
13	M	0.18	0/797	0.39	0/1070
14	N	0.18	0/851	0.36	0/1146
15	O	0.19	0/748	0.45	1/997 (0.1%)
16	P	0.16	0/746	0.38	0/996
17	Q	0.36	1/427 (0.2%)	0.68	1/575 (0.2%)
18	R	0.19	0/531	0.49	0/707
19	S	0.17	0/457	0.40	0/613
20	T	0.18	0/400	0.51	0/536
21	U	0.15	0/370	0.25	0/483
22	V	0.14	0/2152	0.39	0/2902
23	W	0.15	0/3295	0.49	7/4463 (0.2%)
24	Y	0.42	1/1352 (0.1%)	0.90	7/1822 (0.4%)
All	All	0.17	2/88724 (0.0%)	0.36	20/133133 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	W	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	91	PRO	N-CD	5.50	1.55	1.47
24	Y	129	ARG	CA-C	5.50	1.61	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	23	ILE	N-CA-C	-9.64	101.16	110.42
24	Y	54	LYS	N-CA-CB	-8.80	98.42	110.56
24	Y	198	LYS	N-CA-C	-8.61	100.91	111.33
24	Y	54	LYS	N-CA-C	8.46	122.41	112.93
24	Y	61	GLY	N-CA-C	8.07	123.78	110.55
23	W	196	LEU	N-CA-C	-7.94	103.59	113.20
23	W	21	ASN	N-CA-C	6.88	118.43	111.07
3	C	152	GLY	N-CA-C	6.84	129.39	113.18
24	Y	130	VAL	N-CA-CB	6.79	122.44	111.23
23	W	87	ILE	N-CA-C	-6.72	100.30	109.37
3	C	153	GLN	N-CA-C	6.10	118.71	111.33
6	F	149	ILE	N-CA-C	6.05	118.62	111.05
3	C	151	GLY	N-CA-C	5.87	127.09	113.18
24	Y	176	GLY	N-CA-C	5.81	118.01	110.45
17	Q	65	ASP	N-CA-C	5.72	118.17	111.02
24	Y	203	ALA	N-CA-C	-5.67	104.08	111.74
23	W	390	VAL	N-CA-C	-5.45	106.39	111.45
23	W	23	ILE	N-CA-CB	5.42	116.90	110.55
15	O	91	GLU	CA-CB-CG	5.25	124.59	114.10
23	W	88	PHE	N-CA-CB	5.12	118.73	110.65

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	W	391	LYS	Peptide

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	55237	0	27809	804	0
2	B	2395	0	1212	68	0
3	C	1895	0	1985	12	0
4	D	1575	0	1642	15	0
5	E	1551	0	1630	10	0
6	F	1285	0	1246	45	0
7	G	1123	0	1162	1	0
8	H	920	0	977	6	0
9	I	753	0	754	23	0
10	J	953	0	983	7	0
11	K	925	0	995	10	0
12	L	934	0	994	10	0
13	M	786	0	826	8	0
14	N	842	0	899	6	0
15	O	741	0	781	6	0
16	P	737	0	789	5	0
17	Q	423	0	392	13	0
18	R	530	0	568	12	0
19	S	455	0	491	2	0
20	T	394	0	373	7	0
21	U	367	0	410	1	0
22	V	2119	0	2190	31	0
23	W	3239	0	3203	112	0
24	Y	1334	0	1351	126	0
25	V	32	0	13	0	0
25	W	64	0	26	5	0
All	All	81609	0	53701	1241	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 10.

All (1241) 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)
23:W:132:ASP:HA	24:Y:137:MET:CE	1.21	1.59
23:W:132:ASP:CA	24:Y:137:MET:HE1	1.56	1.35
23:W:98:ALA:N	24:Y:52:PRO:HD3	1.48	1.26
23:W:98:ALA:H	24:Y:52:PRO:CD	1.46	1.26
23:W:132:ASP:CA	24:Y:137:MET:CE	2.16	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:116:ALA:HB1	24:Y:121:MET:CE	1.74	1.15
1:A:2152:A:H4'	24:Y:172:HIS:CD2	1.76	1.15
23:W:98:ALA:CB	24:Y:52:PRO:HD3	1.76	1.15
1:A:2206:C:OP1	24:Y:213:ALA:C	1.72	1.14
23:W:180:LEU:HD23	23:W:262:ALA:HB3	1.14	1.13
24:Y:59:ILE:CD1	24:Y:201:PRO:HG2	1.79	1.12
24:Y:59:ILE:HD12	24:Y:201:PRO:HG2	1.34	1.09
23:W:98:ALA:H	24:Y:52:PRO:HD3	1.00	1.09
23:W:132:ASP:HA	24:Y:137:MET:HE3	1.25	1.08
23:W:180:LEU:CD2	23:W:262:ALA:HB3	1.82	1.07
24:Y:116:ALA:HB1	24:Y:121:MET:HE1	1.10	1.06
23:W:98:ALA:CA	24:Y:52:PRO:HD3	1.84	1.05
23:W:97:THR:HG23	24:Y:55:ASN:ND2	1.72	1.04
1:A:1491:A:N6	1:A:1512:G:H1	1.54	1.03
2:B:78:U:H3	2:B:94:G:H1	1.02	0.99
24:Y:59:ILE:CD1	24:Y:201:PRO:CG	2.41	0.98
23:W:98:ALA:HB3	24:Y:52:PRO:CD	1.94	0.97
23:W:97:THR:HG23	24:Y:55:ASN:CG	1.89	0.97
24:Y:116:ALA:CB	24:Y:121:MET:SD	2.52	0.97
24:Y:59:ILE:HD12	24:Y:201:PRO:CG	1.93	0.97
1:A:2152:A:C4'	24:Y:172:HIS:CD2	2.47	0.96
23:W:98:ALA:CB	24:Y:52:PRO:CD	2.44	0.95
24:Y:121:MET:HE2	24:Y:121:MET:HA	1.48	0.95
6:F:3:ARG:HH12	6:F:55:ARG:HD3	1.31	0.95
24:Y:116:ALA:CB	24:Y:121:MET:HE1	1.98	0.94
23:W:98:ALA:CB	24:Y:52:PRO:HG3	1.98	0.94
1:A:1479:G:H1	1:A:1608:A:H61	1.14	0.93
1:A:2353:U:H5"	1:A:2354:G:H5'	1.52	0.92
1:A:2152:A:H4'	24:Y:172:HIS:CG	2.02	0.92
1:A:1527:C:H3'	1:A:1528:U:H5"	1.52	0.91
24:Y:117:THR:O	24:Y:121:MET:SD	2.29	0.90
23:W:98:ALA:H	24:Y:52:PRO:HD2	1.36	0.89
23:W:98:ALA:HB3	24:Y:52:PRO:HD3	1.48	0.88
1:A:2130:G:H1	1:A:2217:U:H3	1.21	0.87
6:F:99:LYS:HB3	6:F:104:LEU:HA	1.56	0.87
24:Y:116:ALA:HB3	24:Y:121:MET:SD	2.12	0.87
23:W:98:ALA:CB	24:Y:52:PRO:CG	2.53	0.87
24:Y:67:ASN:HD21	24:Y:187:GLU:HB2	1.39	0.87
17:Q:76:LYS:HG3	17:Q:90:TYR:HB3	1.56	0.86
24:Y:117:THR:O	24:Y:121:MET:HG2	1.75	0.86
1:A:1479:G:H1	1:A:1608:A:N6	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2207:C:H4'	24:Y:47:ARG:CB	2.06	0.85
1:A:1756:U:H3	1:A:1776:A:H61	1.25	0.84
24:Y:116:ALA:HB1	24:Y:121:MET:SD	2.13	0.84
1:A:1491:A:N7	1:A:1512:G:N2	2.25	0.84
23:W:134:TYR:HD2	24:Y:137:MET:SD	2.01	0.84
1:A:1555:A:H1'	1:A:1556:A:N7	1.92	0.84
23:W:97:THR:HG22	24:Y:52:PRO:CD	2.08	0.83
24:Y:117:THR:O	24:Y:121:MET:CG	2.27	0.83
1:A:1087:U:O2	1:A:1160:G:N2	2.11	0.81
23:W:98:ALA:HB3	24:Y:52:PRO:CG	2.10	0.81
1:A:1094:A:H61	1:A:2780:G:H1	1.23	0.81
23:W:98:ALA:HB3	24:Y:52:PRO:HG3	1.62	0.81
1:A:283:G:N2	1:A:288:C:O2	2.13	0.81
1:A:2207:C:O5'	24:Y:211:ASN:CB	2.29	0.81
23:W:97:THR:HG22	24:Y:52:PRO:N	1.95	0.80
1:A:1096:A:H2'	1:A:1097:A:H4'	1.64	0.80
23:W:132:ASP:HA	24:Y:137:MET:HE1	0.81	0.80
24:Y:67:ASN:HB2	24:Y:188:ASN:HD21	1.47	0.79
1:A:1520:A:H61	1:A:1564:C:H42	1.30	0.78
1:A:303:G:H2'	1:A:304:G:C8	2.19	0.78
1:A:2309:G:N2	1:A:2417:A:C5	2.52	0.78
23:W:132:ASP:C	24:Y:137:MET:HE1	2.09	0.77
1:A:2207:C:C4'	24:Y:47:ARG:CB	2.63	0.77
1:A:202:A:N6	1:A:2463:A:OP2	2.18	0.77
1:A:2207:C:P	24:Y:211:ASN:CB	2.72	0.77
23:W:98:ALA:HB2	24:Y:52:PRO:CG	2.15	0.77
1:A:302:A:O2'	1:A:303:G:N7	2.18	0.77
1:A:2295:A:OP1	1:A:2302:A:N6	2.18	0.76
23:W:197:GLY:O	23:W:198:GLU:HG3	1.84	0.76
1:A:2610:G:H4'	1:A:2611:G:H5'	1.66	0.76
23:W:134:TYR:CD2	24:Y:137:MET:SD	2.80	0.75
24:Y:116:ALA:CB	24:Y:121:MET:CE	2.57	0.75
1:A:2316:A:N7	1:A:2375:A:N6	2.35	0.75
1:A:226:A:H8	1:A:454:G:H21	1.32	0.74
1:A:272:C:N4	1:A:416:U:O4	2.20	0.74
1:A:630:A:H62	1:A:1291:A:H2	1.36	0.74
2:B:38:U:H3	2:B:42:G:H5"	1.53	0.74
23:W:180:LEU:CD2	23:W:262:ALA:CB	2.65	0.74
1:A:1444:C:H2'	1:A:1445:A:H8	1.52	0.74
1:A:1491:A:H62	1:A:1512:G:H1	0.79	0.74
23:W:98:ALA:N	24:Y:52:PRO:CD	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2205:A:H5'	24:Y:214:VAL:C	2.12	0.74
20:T:42:VAL:HB	20:T:47:GLY:HA2	1.69	0.74
23:W:98:ALA:HB2	24:Y:52:PRO:HG3	1.67	0.73
23:W:132:ASP:CA	24:Y:137:MET:HE3	2.02	0.73
2:B:35:C:H42	2:B:46:A:H4'	1.53	0.73
2:B:75:U:O2'	2:B:76:A:N7	2.20	0.72
1:A:1340:A:H2	1:A:1671:G:H21	1.34	0.72
1:A:283:G:N2	1:A:289:C:O2	2.22	0.72
1:A:2104:U:N3	1:A:2106:A:N7	2.36	0.72
1:A:2777:A:N7	1:A:2783:U:O2	2.23	0.72
1:A:2273:U:H2'	1:A:2274:U:H6	1.54	0.72
1:A:847:A:H4'	1:A:848:G:H5'	1.71	0.72
1:A:2138:U:H2'	1:A:2139:G:C8	2.26	0.71
1:A:303:G:H2'	1:A:304:G:H8	1.53	0.70
1:A:309:U:H4'	1:A:407:A:H62	1.55	0.70
24:Y:200:LYS:HE3	24:Y:201:PRO:HD2	1.73	0.70
1:A:1246:G:H1'	1:A:1247:G:H5'	1.73	0.70
24:Y:121:MET:HE2	24:Y:121:MET:CA	2.20	0.70
1:A:2309:G:N2	1:A:2417:A:C6	2.59	0.70
20:T:48:SER:HA	20:T:53:ASP:HA	1.72	0.70
1:A:2125:U:H2'	1:A:2126:G:H8	1.57	0.69
2:B:42:G:N3	2:B:45:C:N4	2.39	0.69
23:W:97:THR:CG2	24:Y:55:ASN:ND2	2.53	0.69
24:Y:201:PRO:HG2	24:Y:208:TYR:HE1	1.57	0.69
1:A:1497:G:N1	1:A:1505:U:N3	2.38	0.69
1:A:327:G:H1	1:A:400:U:H3	1.40	0.69
1:A:2776:G:H21	1:A:2786:A:H62	1.38	0.69
23:W:176:ILE:HD11	23:W:225:PHE:HE1	1.57	0.69
1:A:732:A:H8	1:A:735:U:H3	1.39	0.69
2:B:15:C:H3'	2:B:16:G:H8	1.58	0.69
11:K:112:ARG:HH12	11:K:114:LYS:HA	1.58	0.69
24:Y:67:ASN:HB2	24:Y:188:ASN:ND2	2.08	0.69
6:F:61:GLU:N	6:F:61:GLU:OE1	2.26	0.68
1:A:430:C:N4	1:A:433:G:OP1	2.26	0.68
1:A:1482:G:H21	1:A:1562:A:H8	1.41	0.68
23:W:266:ASP:OD2	23:W:269:GLU:HB3	1.92	0.68
6:F:72:LEU:O	6:F:75:ASN:HB2	1.92	0.68
1:A:1094:A:N6	1:A:2780:G:H1	1.91	0.68
1:A:2824:G:N2	1:A:2826:A:OP2	2.26	0.68
23:W:234:ARG:HG2	23:W:235:LYS:H	1.58	0.68
1:A:2206:C:OP1	24:Y:214:VAL:N	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2309:G:C2	1:A:2417:A:C6	2.81	0.68
1:A:1479:G:N2	1:A:1608:A:N1	2.42	0.68
1:A:300:G:H4'	1:A:301:U:H5'	1.76	0.67
1:A:1347:A:H62	1:A:1651:G:H8	1.43	0.67
9:I:23:ILE:HD11	13:M:81:ASN:HB3	1.76	0.67
1:A:2688:G:N2	1:A:2691:A:OP2	2.27	0.67
24:Y:59:ILE:HG21	24:Y:208:TYR:OH	1.95	0.67
1:A:1074:A:OP1	2:B:85:U:O2'	2.13	0.66
1:A:1479:G:H2'	1:A:1480:A:N3	2.10	0.66
24:Y:59:ILE:CD1	24:Y:201:PRO:HG3	2.24	0.66
1:A:2310:C:O2'	1:A:2418:G:N3	2.28	0.66
1:A:1556:A:H2'	1:A:1557:G:O4'	1.94	0.66
23:W:234:ARG:HG2	23:W:235:LYS:N	2.10	0.66
1:A:698:C:H3'	1:A:699:A:C8	2.31	0.66
1:A:2357:A:N6	1:A:2416:U:O2	2.18	0.66
24:Y:199:ALA:O	24:Y:201:PRO:HD3	1.95	0.66
1:A:872:C:H4'	1:A:2457:G:C6	2.31	0.66
1:A:2557:U:H3	1:A:2564:G:H1	1.41	0.66
1:A:1087:U:N3	1:A:1160:G:N1	2.41	0.66
1:A:2426:G:O6	1:A:2448:U:O2	2.14	0.66
24:Y:101:ILE:HD11	24:Y:124:VAL:HG23	1.79	0.65
1:A:1496:G:H1	1:A:1507:U:H3	1.42	0.65
1:A:2823:C:H3'	1:A:2824:G:H8	1.61	0.65
1:A:683:A:C5	1:A:698:C:H1'	2.31	0.65
1:A:910:A:O2'	2:B:98:G:N3	2.30	0.65
2:B:110:G:H3'	2:B:111:C:H5"	1.78	0.65
1:A:1444:C:H2'	1:A:1445:A:C8	2.31	0.64
24:Y:66:PRO:C	24:Y:68:GLY:H	2.05	0.64
1:A:282:G:N2	1:A:283:G:O6	2.30	0.64
23:W:183:ARG:NH2	23:W:266:ASP:OD2	2.31	0.64
1:A:1268:G:OP2	12:L:12:LYS:NZ	2.28	0.64
2:B:79:C:H2'	2:B:80:G:C8	2.32	0.64
1:A:1242:U:H2'	1:A:1243:A:H8	1.63	0.64
1:A:267:C:O2'	1:A:268:A:O5'	2.14	0.63
1:A:2318:G:O2'	1:A:2375:A:N7	2.29	0.63
1:A:761:U:H2'	1:A:762:A:H3'	1.78	0.63
24:Y:194:ASP:HA	24:Y:197:LEU:HG	1.80	0.63
1:A:296:G:O2'	1:A:297:G:OP1	2.17	0.63
1:A:316:G:H2'	1:A:317:G:C8	2.32	0.63
1:A:617:G:N1	1:A:2060:A:OP1	2.27	0.63
1:A:414:C:O2'	1:A:415:C:OP1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:G:O6	1:A:444:U:O2	2.15	0.63
1:A:966:U:H3'	1:A:967:G:H8	1.63	0.63
1:A:2152:A:C4'	24:Y:172:HIS:CG	2.78	0.63
1:A:2370:G:H22	1:A:2404:G:H5"	1.63	0.63
23:W:176:ILE:HD11	23:W:225:PHE:CE1	2.33	0.63
1:A:905:G:N2	1:A:2298:A:OP2	2.30	0.63
1:A:2440:A:N6	1:A:2441:A:N3	2.47	0.63
1:A:2695:C:H4'	6:F:110:TYR:CZ	2.34	0.63
24:Y:80:LYS:NZ	24:Y:120:MET:HB2	2.14	0.63
1:A:693:G:N3	1:A:2379:C:O2'	2.32	0.62
24:Y:195:THR:HA	24:Y:198:LYS:HE2	1.80	0.62
13:M:50:ASN:HB2	13:M:51:PRO:HD3	1.80	0.62
1:A:1220:G:H2'	1:A:1221:A:H8	1.63	0.62
2:B:74:G:N1	2:B:99:A:C2	2.68	0.62
1:A:1759:U:OP1	1:A:1773:G:N1	2.32	0.62
6:F:3:ARG:NH1	6:F:55:ARG:HD3	2.09	0.62
2:B:6:U:O2	2:B:110:G:O6	2.18	0.62
1:A:2488:A:N6	1:A:2525:C:O2	2.30	0.62
2:B:70:G:N2	2:B:102:A:OP2	2.33	0.61
1:A:2455:A:O2'	1:A:2458:G:OP1	2.17	0.61
1:A:437:A:H2'	1:A:438:A:H8	1.64	0.61
1:A:445:C:O2'	1:A:446:G:O5'	2.18	0.61
1:A:1025:A:H5'	1:A:1026:A:H5"	1.82	0.61
1:A:1093:G:N2	1:A:1157:A:OP2	2.29	0.61
2:B:4:G:H5'	2:B:25:A:H2	1.65	0.61
1:A:874:U:O2	1:A:2459:A:N6	2.33	0.61
1:A:1069:U:OP2	1:A:1071:G:N2	2.33	0.61
1:A:2305:G:H2'	1:A:2306:G:C8	2.35	0.61
1:A:2091:A:N6	1:A:2639:C:N3	2.49	0.61
1:A:2272:U:O2'	1:A:2273:U:OP1	2.18	0.61
24:Y:78:PHE:HB3	24:Y:120:MET:HE3	1.81	0.61
24:Y:201:PRO:HD2	24:Y:208:TYR:CE1	2.35	0.61
1:A:305:A:H62	1:A:411:G:H21	1.49	0.61
1:A:722:A:OP1	5:E:63:LYS:NZ	2.32	0.61
1:A:2265:U:H3'	1:A:2266:G:C8	2.36	0.61
1:A:2321:U:H2'	1:A:2322:C:C6	2.35	0.61
1:A:1374:C:OP1	15:O:65:ARG:NH1	2.34	0.61
1:A:1491:A:N6	1:A:1512:G:N1	2.28	0.61
1:A:2292:C:N4	1:A:2306:G:O6	2.34	0.61
1:A:510:G:N2	1:A:513:A:OP2	2.27	0.60
1:A:2435:C:N4	1:A:2438:G:N7	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:C:H3'	2:B:29:C:H6	1.66	0.60
1:A:326:A:H3'	1:A:327:G:H5"	1.83	0.60
1:A:2295:A:N6	1:A:2302:A:OP2	2.34	0.60
23:W:393:PRO:HG3	23:W:423:PHE:CE1	2.36	0.60
1:A:1811:C:O2	1:A:2637:G:O2'	2.16	0.60
1:A:2292:C:O2'	1:A:2293:C:OP1	2.18	0.60
2:B:4:G:H5'	2:B:25:A:C2	2.37	0.60
2:B:28:C:O2'	2:B:56:A:N7	2.33	0.60
1:A:275:A:N7	1:A:296:G:N2	2.48	0.60
1:A:2309:G:N3	1:A:2417:A:C6	2.70	0.60
2:B:14:G:H2'	2:B:15:C:H6	1.67	0.60
1:A:1096:A:N6	1:A:1097:A:N3	2.49	0.60
1:A:617:G:N2	1:A:2060:A:OP2	2.34	0.60
1:A:2090:G:N2	1:A:2092:C:O4'	2.34	0.60
11:K:104:ARG:O	11:K:107:ARG:NH2	2.35	0.60
1:A:2122:G:N2	1:A:2226:U:O2	2.34	0.59
1:A:459:A:N6	1:A:2442:G:OP1	2.34	0.59
1:A:1094:A:N6	1:A:2780:G:N1	2.39	0.59
1:A:297:G:H2'	1:A:298:U:C6	2.38	0.59
1:A:2153:G:H5'	24:Y:43:GLU:OE2	2.03	0.59
6:F:149:ILE:HD12	6:F:149:ILE:H	1.67	0.59
1:A:872:C:H2'	1:A:873:U:C6	2.37	0.59
1:A:2267:G:H4'	1:A:2268:G:OP2	2.03	0.59
2:B:11:A:H1'	2:B:14:G:H1'	1.83	0.59
6:F:105:VAL:HG22	6:F:115:GLU:HG3	1.84	0.59
20:T:31:PRO:HB3	20:T:50:ASN:N	2.18	0.59
23:W:197:GLY:O	23:W:198:GLU:CG	2.50	0.59
1:A:305:A:H2'	1:A:306:C:H5'	1.83	0.59
1:A:1783:C:H5	11:K:97:ARG:HH21	1.49	0.59
1:A:1458:U:H1'	1:A:1460:G:C6	2.38	0.59
3:C:145:GLU:HB3	3:C:188:CYS:HB3	1.84	0.59
1:A:2273:U:H2'	1:A:2274:U:C6	2.36	0.58
1:A:965:A:N3	2:B:78:U:O2'	2.36	0.58
1:A:1362:G:O2'	1:A:1363:G:OP1	2.17	0.58
1:A:2351:A:O2'	1:A:2352:G:OP1	2.19	0.58
6:F:22:ASN:O	6:F:37:THR:OG1	2.20	0.58
1:A:1497:G:O6	1:A:1505:U:O4	2.22	0.58
1:A:2326:C:H3'	1:A:2327:A:C8	2.38	0.58
1:A:309:U:H4'	1:A:407:A:N6	2.19	0.58
1:A:1097:A:N6	1:A:1156:G:N3	2.51	0.58
23:W:266:ASP:OD1	23:W:266:ASP:O	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2374:G:O6	1:A:2400:G:O6	2.20	0.58
1:A:2453:C:O2'	1:A:2458:G:N2	2.37	0.58
13:M:99:LYS:HG3	13:M:101:ASN:HB2	1.84	0.58
22:V:124:LEU:HD13	22:V:170:LEU:HD23	1.86	0.58
1:A:2152:A:C5'	24:Y:172:HIS:CD2	2.87	0.58
1:A:2560:A:N6	1:A:2691:A:H61	2.02	0.58
1:A:2195:G:H1	1:A:2200:A:H3'	1.67	0.58
1:A:2561:G:O2'	1:A:2686:A:N1	2.36	0.58
1:A:2778:A:OP2	1:A:2779:A:O2'	2.21	0.58
24:Y:80:LYS:HZ2	24:Y:120:MET:HB2	1.67	0.58
1:A:5:A:H2'	1:A:6:A:C8	2.39	0.57
1:A:2408:G:H2'	1:A:2409:U:H6	1.69	0.57
6:F:18:THR:HG22	6:F:26:ALA:HB3	1.85	0.57
16:P:93:VAL:HG12	16:P:100:VAL:HA	1.84	0.57
24:Y:59:ILE:HD12	24:Y:201:PRO:HG3	1.81	0.57
1:A:2309:G:C2	1:A:2417:A:N1	2.72	0.57
6:F:138:ASP:HB2	6:F:141:ARG:HG2	1.86	0.57
1:A:1310:C:H5"	1:A:1311:G:H5'	1.87	0.57
1:A:2405:A:H2'	1:A:2406:A:C8	2.39	0.57
1:A:1568:G:N2	1:A:1569:A:O2'	2.38	0.57
2:B:69:C:H2'	2:B:70:G:O4'	2.04	0.57
24:Y:101:ILE:CD1	24:Y:124:VAL:HG23	2.33	0.57
1:A:906:G:H1'	1:A:907:U:H5	1.69	0.57
1:A:1478:G:H2'	1:A:1479:G:C8	2.40	0.57
5:E:132:ASP:OD1	5:E:133:THR:N	2.38	0.57
1:A:2408:G:H2'	1:A:2409:U:C6	2.40	0.57
23:W:26:GLU:HG2	23:W:250:ARG:HH22	1.70	0.57
1:A:896:A:H2'	1:A:897:G:H8	1.70	0.57
1:A:2090:G:H4'	1:A:2091:A:OP1	2.04	0.57
8:H:63:VAL:HG21	8:H:102:VAL:HG22	1.86	0.57
23:W:44:SER:OG	23:W:45:SER:N	2.38	0.57
1:A:1460:G:N2	1:A:1631:A:C5	2.72	0.57
1:A:2374:G:H8	1:A:2376:C:H41	1.51	0.57
1:A:2553:G:H1	1:A:2568:C:H41	1.52	0.57
4:D:100:GLU:N	4:D:100:GLU:OE1	2.38	0.57
9:I:90:GLU:OE1	9:I:92:THR:N	2.38	0.57
23:W:33:ASP:HB2	23:W:35:PRO:HD2	1.86	0.57
24:Y:121:MET:HA	24:Y:124:VAL:HG12	1.87	0.57
1:A:688:G:H4'	1:A:692:A:H62	1.70	0.57
1:A:2059:A:H4'	1:A:2060:A:C8	2.40	0.57
1:A:259:A:H2'	1:A:260:A:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:A:H2'	1:A:279:A:H8	1.69	0.56
2:B:71:A:OP2	2:B:100:G:N1	2.34	0.56
24:Y:59:ILE:HD11	24:Y:201:PRO:HG2	1.79	0.56
1:A:279:A:H2'	1:A:280:G:C8	2.40	0.56
1:A:342:A:N3	1:A:363:C:O2'	2.38	0.56
1:A:462:A:O2'	1:A:463:U:OP1	2.22	0.56
24:Y:49:GLY:HA2	24:Y:210:LYS:HE3	1.87	0.56
1:A:350:U:O2'	1:A:1251:U:OP1	2.23	0.56
1:A:2576:U:O2'	1:A:2577:G:O5'	2.23	0.56
1:A:2858:U:H4'	1:A:2859:G:O5'	2.05	0.56
2:B:98:G:H3'	2:B:99:A:H8	1.70	0.56
18:R:10:THR:O	18:R:13:GLU:HG3	2.05	0.56
1:A:89:U:H2'	1:A:90:A:C8	2.41	0.56
1:A:2308:G:N2	1:A:2356:A:N3	2.54	0.56
2:B:66:C:H2'	2:B:67:G:H5'	1.86	0.56
23:W:116:LEU:HD11	23:W:136:LEU:HD12	1.86	0.56
1:A:2473:G:OP1	5:E:74:ARG:NH1	2.38	0.56
1:A:823:G:H3'	1:A:824:G:H5'	1.88	0.56
1:A:1556:A:H3'	1:A:1557:G:C8	2.40	0.56
24:Y:197:LEU:O	24:Y:198:LYS:C	2.47	0.56
1:A:869:U:N3	1:A:870:A:N7	2.53	0.56
1:A:2414:C:O2	17:Q:49:ARG:NH2	2.39	0.56
23:W:21:ASN:HD22	23:W:30:ILE:HD11	1.71	0.56
24:Y:201:PRO:CD	24:Y:208:TYR:CE1	2.88	0.56
1:A:288:C:H2'	1:A:289:C:C2	2.40	0.56
1:A:288:C:O2'	1:A:289:C:OP1	2.24	0.56
1:A:2780:G:H3'	1:A:2781:C:H6	1.71	0.56
23:W:41:ARG:HG2	23:W:58:THR:HG22	1.87	0.56
1:A:682:G:OP2	9:I:129:SER:OG	2.20	0.56
1:A:2882:G:N2	1:A:2885:A:OP2	2.34	0.56
1:A:1774:A:H3'	1:A:1775:G:H8	1.70	0.56
1:A:1837:U:O2'	1:A:1838:A:OP1	2.22	0.56
5:E:117:LYS:NZ	5:E:186:VAL:O	2.37	0.56
1:A:1213:G:H2'	1:A:1214:U:C6	2.41	0.55
22:V:29:GLU:OE1	22:V:53:ARG:NH1	2.39	0.55
1:A:5:A:H2'	1:A:6:A:H8	1.72	0.55
1:A:198:A:H62	1:A:201:C:P	2.30	0.55
1:A:465:U:H2'	1:A:466:C:C6	2.42	0.55
1:A:1001:U:O4	1:A:1004:U:O2'	2.23	0.55
1:A:1465:A:H2'	1:A:1467:G:N7	2.21	0.55
1:A:911:G:O2'	1:A:912:C:H5'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1527:C:H2'	1:A:1528:U:C6	2.41	0.55
4:D:6:LEU:HD21	4:D:81:LYS:CG	2.36	0.55
1:A:1526:G:C2	1:A:1559:C:C2	2.94	0.55
1:A:2405:A:O2'	1:A:2406:A:OP1	2.22	0.55
23:W:62:ASP:O	23:W:73:ARG:NH2	2.37	0.55
1:A:1065:U:H3	1:A:1188:A:H62	1.54	0.55
1:A:2131:U:H2'	1:A:2132:A:C8	2.42	0.55
1:A:2197:G:H2'	1:A:2198:G:N2	2.20	0.55
1:A:2104:U:O2'	1:A:2105:U:H5'	2.05	0.55
9:I:90:GLU:OE1	9:I:92:THR:HG23	2.06	0.55
1:A:316:G:H2'	1:A:317:G:H8	1.70	0.55
1:A:2102:C:O2	1:A:2465:G:N2	2.39	0.55
1:A:2322:C:H2'	1:A:2323:C:C5	2.41	0.55
24:Y:73:GLN:O	24:Y:157:LYS:NZ	2.39	0.55
1:A:2628:G:O2'	1:A:2629:A:H8	1.90	0.55
2:B:14:G:H2'	2:B:15:C:C6	2.42	0.55
18:R:8:ASP:OD1	18:R:9:LEU:N	2.40	0.55
23:W:97:THR:HG22	24:Y:52:PRO:HD2	1.87	0.55
1:A:303:G:O2'	1:A:304:G:OP1	2.24	0.55
1:A:349:C:H2'	1:A:350:U:C6	2.42	0.55
1:A:792:G:O2'	1:A:795:G:O2'	2.23	0.55
1:A:2467:U:H2'	1:A:2470:C:C5	2.42	0.54
1:A:2686:A:O4'	1:A:2694:A:N6	2.40	0.54
2:B:22:G:H5"	2:B:24:C:H41	1.72	0.54
1:A:682:G:N7	9:I:110:LYS:NZ	2.53	0.54
1:A:1082:G:O6	1:A:1165:U:O2	2.25	0.54
1:A:309:U:O2'	1:A:407:A:N7	2.39	0.54
1:A:1250:G:H5"	1:A:1251:U:H3'	1.89	0.54
1:A:1694:G:O2'	10:J:110:ASP:OD2	2.25	0.54
1:A:2291:U:N3	1:A:2308:G:N7	2.56	0.54
1:A:2309:G:N3	1:A:2417:A:N1	2.54	0.54
6:F:45:LYS:HE2	6:F:52:THR:HG23	1.89	0.54
1:A:2712:C:OP1	11:K:54:ARG:NH2	2.38	0.54
1:A:2788:G:N2	6:F:140:GLU:OE2	2.40	0.54
23:W:32:GLU:OE2	23:W:32:GLU:N	2.40	0.54
23:W:97:THR:HG23	24:Y:55:ASN:CB	2.36	0.54
1:A:2783:U:O2'	1:A:2785:U:OP1	2.18	0.54
1:A:2911:G:H2'	1:A:2912:A:H8	1.71	0.54
9:I:117:LEU:HD12	9:I:118:GLU:H	1.71	0.54
1:A:278:A:H2'	1:A:279:A:C8	2.43	0.54
1:A:2777:A:H2'	1:A:2778:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2360:G:H21	1:A:2365:A:H2	1.54	0.54
2:B:70:G:H22	2:B:101:U:H3'	1.72	0.54
2:B:76:A:H2'	2:B:77:G:O4'	2.08	0.54
24:Y:175:ILE:HB	24:Y:188:ASN:HB3	1.89	0.54
1:A:687:U:H3'	1:A:688:G:C8	2.43	0.54
1:A:1426:A:H5'	1:A:1515:C:H1'	1.90	0.54
1:A:2109:G:O2'	1:A:2110:C:OP1	2.25	0.54
1:A:2582:G:C6	1:A:2584:U:H5'	2.42	0.54
6:F:85:GLU:O	6:F:86:ARG:HD2	2.07	0.54
24:Y:121:MET:CE	24:Y:121:MET:CA	2.86	0.54
1:A:2295:A:H4'	1:A:2296:A:H5"	1.90	0.54
22:V:266:ASP:OD1	22:V:267:ILE:N	2.41	0.54
24:Y:59:ILE:HD13	24:Y:201:PRO:CG	2.34	0.54
24:Y:104:ILE:HA	24:Y:108:TRP:HB2	1.90	0.54
1:A:1516:A:H62	1:A:1568:G:H8	1.55	0.53
1:A:1527:C:H3'	1:A:1528:U:C5'	2.32	0.53
1:A:1528:U:H4'	1:A:1529:G:H4'	1.90	0.53
1:A:2149:G:H2'	1:A:2150:G:C8	2.43	0.53
2:B:44:A:H2'	2:B:45:C:O4'	2.08	0.53
22:V:27:VAL:HG11	22:V:48:LEU:HD11	1.89	0.53
1:A:1074:A:H2'	1:A:1075:A:H8	1.73	0.53
1:A:1075:A:H3'	1:A:1076:G:H8	1.74	0.53
1:A:2318:G:H2'	1:A:2319:G:N7	2.24	0.53
1:A:1859:C:O2'	1:A:1860:G:H8	1.91	0.53
6:F:59:GLN:HG3	6:F:61:GLU:OE1	2.09	0.53
18:R:11:THR:HA	18:R:14:ILE:HD12	1.91	0.53
18:R:20:SER:O	18:R:24:GLU:HG3	2.08	0.53
1:A:198:A:H3'	1:A:199:A:H4'	1.91	0.53
1:A:692:A:H3'	1:A:693:G:H8	1.74	0.53
3:C:5:LYS:HG2	3:C:17:THR:HG22	1.89	0.53
17:Q:76:LYS:HG2	17:Q:90:TYR:H	1.73	0.53
1:A:1002:G:O6	1:A:1004:U:O2'	2.23	0.53
1:A:1455:C:O2'	1:A:1456:A:OP1	2.26	0.53
1:A:1540:A:H2'	1:A:1541:A:C8	2.44	0.53
1:A:275:A:H61	1:A:297:G:H1'	1.72	0.53
1:A:439:U:O2'	1:A:440:U:OP1	2.25	0.53
4:D:180:ASP:OD1	4:D:185:LEU:HB2	2.08	0.53
24:Y:117:THR:N	24:Y:121:MET:SD	2.82	0.53
1:A:513:A:OP1	21:U:34:ARG:NH1	2.42	0.53
1:A:1214:U:H2'	1:A:1215:U:C6	2.44	0.53
1:A:1448:U:O2	1:A:1449:C:N4	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:28:GLU:N	13:M:31:GLU:OE1	2.41	0.53
1:A:106:G:H1'	1:A:337:A:H8	1.73	0.53
1:A:1656:C:O2'	1:A:1657:C:O5'	2.27	0.53
6:F:3:ARG:O	6:F:7:LYS:NZ	2.42	0.53
1:A:63:G:H21	15:O:66:VAL:HG11	1.74	0.53
1:A:874:U:N3	1:A:2459:A:N1	2.54	0.53
1:A:1245:G:H1'	1:A:1246:G:H5'	1.90	0.53
1:A:2201:U:H1'	1:A:2203:C:C2	2.43	0.53
1:A:2357:A:H2'	1:A:2358:A:C8	2.44	0.53
1:A:2457:G:H4'	1:A:2458:G:C5	2.44	0.53
1:A:252:C:OP1	1:A:2423:C:H4'	2.10	0.52
1:A:2022:U:H2'	1:A:2023:C:H5'	1.90	0.52
6:F:45:LYS:H	6:F:53:VAL:HG22	1.73	0.52
1:A:284:C:HO2'	1:A:288:C:HO2'	1.58	0.52
1:A:2403:C:N4	1:A:2404:G:O6	2.42	0.52
1:A:626:G:H2'	1:A:627:G:H8	1.73	0.52
1:A:1018:G:H3'	1:A:1019:A:H5"	1.92	0.52
23:W:292:VAL:HG13	23:W:328:MET:HE1	1.92	0.52
1:A:58:G:O2'	1:A:59:G:OP1	2.26	0.52
1:A:1074:A:H2'	1:A:1075:A:C8	2.44	0.52
1:A:1339:A:H4'	1:A:1340:A:O5'	2.09	0.52
23:W:197:GLY:C	23:W:198:GLU:HG3	2.34	0.52
1:A:2062:A:O2'	1:A:2064:G:OP2	2.22	0.52
1:A:2123:A:N6	1:A:2224:U:O4	2.43	0.52
23:W:302:ASP:O	23:W:305:THR:OG1	2.26	0.52
1:A:416:U:O2'	1:A:470:A:OP2	2.25	0.52
1:A:264:G:C2	1:A:265:A:C8	2.98	0.52
1:A:867:A:H4'	1:A:883:G:N2	2.24	0.52
1:A:2323:C:O2'	1:A:2324:C:OP1	2.24	0.52
2:B:102:A:H3'	2:B:103:G:H8	1.75	0.52
1:A:2421:A:H5"	1:A:2423:C:H41	1.75	0.52
22:V:191:VAL:HG22	22:V:205:VAL:HG13	1.92	0.52
1:A:902:G:O6	1:A:970:A:N6	2.43	0.52
6:F:110:TYR:HD1	6:F:112:HIS:CD2	2.29	0.52
6:F:149:ILE:HD12	6:F:149:ILE:N	2.25	0.52
1:A:314:A:H1'	1:A:316:G:C2	2.46	0.51
1:A:1438:C:O2'	1:A:1439:U:OP1	2.28	0.51
1:A:1519:C:H42	1:A:1565:U:H3	1.58	0.51
1:A:1782:G:N2	1:A:1785:G:OP2	2.41	0.51
10:J:91:TYR:OH	10:J:120:VAL:O	2.21	0.51
14:N:73:GLN:HB2	14:N:106:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:53:ARG:NH1	22:V:55:MET:SD	2.83	0.51
23:W:234:ARG:CG	23:W:235:LYS:H	2.23	0.51
23:W:396:VAL:HG22	23:W:431:PHE:HB3	1.92	0.51
1:A:314:A:H1'	1:A:316:G:C4	2.45	0.51
1:A:674:G:H2'	1:A:675:C:C6	2.44	0.51
1:A:688:G:C2	1:A:690:A:H5"	2.44	0.51
1:A:698:C:H2'	1:A:698:C:O2	2.11	0.51
3:C:39:LYS:NZ	3:C:57:GLY:O	2.42	0.51
1:A:871:G:O2'	1:A:872:C:H5"	2.11	0.51
9:I:110:LYS:HG3	9:I:127:LYS:HG3	1.93	0.51
23:W:364:MET:HA	23:W:367:VAL:HG12	1.90	0.51
24:Y:120:MET:O	24:Y:120:MET:HG2	2.10	0.51
1:A:1480:A:H62	1:A:1606:A:H61	1.59	0.51
1:A:2124:A:H2'	1:A:2125:U:C6	2.45	0.51
1:A:2582:G:C5	1:A:2584:U:H5'	2.46	0.51
4:D:146:MET:HG2	4:D:158:LYS:HE2	1.92	0.51
1:A:304:G:H2'	1:A:305:A:C8	2.45	0.51
1:A:907:U:HO2'	1:A:908:A:H8	1.56	0.51
1:A:2150:G:O2'	1:A:2151:U:OP1	2.29	0.51
1:A:2209:U:H2'	1:A:2210:G:C8	2.45	0.51
23:W:162:HIS:O	23:W:164:LYS:NZ	2.39	0.51
1:A:461:C:HO2'	1:A:462:A:H8	1.59	0.51
1:A:637:A:H2'	1:A:638:U:C6	2.46	0.51
1:A:906:G:N2	1:A:907:U:O4	2.36	0.51
1:A:2193:C:H3'	1:A:2194:G:H8	1.76	0.51
1:A:2313:C:C2	1:A:2413:G:N2	2.79	0.51
1:A:403:C:H2'	1:A:404:C:C6	2.46	0.51
1:A:1096:A:C6	1:A:1097:A:H1'	2.46	0.51
1:A:2404:G:N2	1:A:2406:A:H3'	2.26	0.51
1:A:2429:G:H2'	1:A:2430:U:C6	2.46	0.51
1:A:2694:A:H5"	1:A:2695:C:C5	2.46	0.51
1:A:1220:G:H2'	1:A:1221:A:C8	2.45	0.51
1:A:2296:A:H8	1:A:2300:G:H1	1.58	0.51
1:A:2298:A:H3'	1:A:2299:G:H8	1.76	0.51
1:A:2909:U:H2'	1:A:2910:C:O4'	2.11	0.51
2:B:75:U:O3'	2:B:97:A:N6	2.43	0.51
23:W:266:ASP:CG	23:W:269:GLU:HB3	2.36	0.51
24:Y:66:PRO:O	24:Y:68:GLY:N	2.44	0.51
1:A:313:U:H4'	1:A:314:A:H5"	1.92	0.51
1:A:327:G:OP1	1:A:327:G:H4'	2.09	0.51
1:A:1315:G:OP2	1:A:1690:G:O2'	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1618:A:H2'	1:A:1619:A:C8	2.46	0.51
1:A:688:G:N3	1:A:690:A:H5"	2.26	0.50
1:A:2132:A:H2'	1:A:2133:C:C6	2.45	0.50
1:A:2155:A:N6	24:Y:39:ASP:N	2.59	0.50
1:A:2380:G:H1'	1:A:2396:G:N2	2.26	0.50
1:A:870:A:C2'	1:A:871:G:H5'	2.40	0.50
1:A:1263:G:N7	13:M:70:LYS:NZ	2.60	0.50
23:W:319:PHE:CZ	23:W:320:LEU:HD22	2.46	0.50
24:Y:67:ASN:ND2	24:Y:67:ASN:H	2.08	0.50
1:A:172:U:H2'	1:A:173:A:H8	1.74	0.50
1:A:906:G:H22	1:A:964:A:P	2.34	0.50
1:A:2138:U:H3	1:A:2209:U:H3	1.60	0.50
23:W:333:LYS:O	23:W:333:LYS:HG2	2.10	0.50
1:A:198:A:C5	1:A:200:A:H5'	2.45	0.50
1:A:1213:G:H2'	1:A:1214:U:H6	1.76	0.50
1:A:2857:U:OP1	4:D:59:LYS:NZ	2.43	0.50
23:W:25:GLY:HA3	23:W:27:ARG:CZ	2.41	0.50
1:A:896:A:H2'	1:A:897:G:C8	2.45	0.50
1:A:1000:G:H22	1:A:1009:U:H3	1.58	0.50
1:A:1093:G:H2'	1:A:1157:A:N6	2.26	0.50
1:A:1476:C:H2'	1:A:1477:A:C8	2.46	0.50
1:A:2149:G:H2'	1:A:2150:G:H8	1.77	0.50
6:F:104:LEU:N	6:F:116:ILE:O	2.42	0.50
1:A:699:A:H2'	1:A:700:U:C5	2.46	0.50
1:A:1496:G:H22	1:A:1507:U:H3	1.58	0.50
1:A:1774:A:H3'	1:A:1775:G:C8	2.47	0.50
1:A:2128:U:H1'	1:A:2220:A:C2	2.46	0.50
5:E:32:VAL:HG12	5:E:109:ALA:HB2	1.94	0.50
9:I:71:ARG:HB3	9:I:73:GLU:OE2	2.11	0.50
1:A:90:A:H4'	1:A:91:A:O5'	2.12	0.50
1:A:200:A:H5"	1:A:201:C:C5	2.46	0.50
1:A:692:A:N1	1:A:2379:C:H1'	2.27	0.50
22:V:206:ALA:HB2	22:V:260:THR:HG23	1.94	0.50
1:A:78:U:H2'	1:A:79:C:C6	2.47	0.50
1:A:675:C:H2'	1:A:676:G:H8	1.77	0.50
1:A:1515:C:H2'	1:A:1516:A:H8	1.77	0.50
1:A:2198:G:H2'	1:A:2199:G:C4	2.46	0.50
1:A:2610:G:H8	1:A:2612:G:N7	2.10	0.50
1:A:2647:G:H21	4:D:146:MET:HE1	1.75	0.50
2:B:15:C:H2'	2:B:16:G:O4'	2.11	0.50
2:B:112:C:H2'	2:B:113:A:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:72:ALA:HB2	4:D:93:VAL:HG12	1.93	0.50
22:V:122:ARG:HG2	22:V:168:GLU:HB2	1.93	0.50
24:Y:65:LEU:HD13	24:Y:66:PRO:HD2	1.94	0.50
24:Y:121:MET:SD	24:Y:145:VAL:HG13	2.52	0.50
1:A:626:G:H2'	1:A:627:G:C8	2.47	0.50
1:A:2494:C:H2'	1:A:2495:C:C6	2.47	0.50
1:A:873:U:H3	1:A:879:G:H1	1.59	0.49
1:A:2313:C:O2	1:A:2354:G:N1	2.45	0.49
1:A:2585:C:H4'	1:A:2586:G:O5'	2.12	0.49
2:B:26:C:C2	2:B:27:A:H1'	2.46	0.49
2:B:100:G:H2'	2:B:101:U:C6	2.47	0.49
9:I:96:LEU:HB2	9:I:102:ILE:HG22	1.94	0.49
16:P:69:MET:SD	16:P:78:VAL:HB	2.52	0.49
18:R:36:GLN:N	18:R:36:GLN:OE1	2.45	0.49
1:A:201:C:H2'	1:A:202:A:H2'	1.93	0.49
1:A:2318:G:H2'	1:A:2319:G:C8	2.47	0.49
2:B:3:U:H3	2:B:113:A:H2	1.60	0.49
4:D:98:LYS:HB3	4:D:100:GLU:OE1	2.11	0.49
14:N:28:GLN:HB2	14:N:31:GLU:HG3	1.94	0.49
1:A:115:C:O2'	1:A:125:A:N3	2.44	0.49
1:A:1491:A:N6	1:A:1512:G:C6	2.80	0.49
1:A:2409:U:O2'	1:A:2410:C:OP1	2.28	0.49
1:A:462:A:H2'	1:A:463:U:C6	2.47	0.49
1:A:805:G:H21	1:A:2010:A:H62	1.60	0.49
1:A:1019:A:OP1	1:A:1019:A:H8	1.95	0.49
1:A:1092:A:O3'	1:A:1093:G:H8	1.95	0.49
1:A:1477:A:H2'	1:A:1478:G:C8	2.48	0.49
1:A:1528:U:C4'	1:A:1529:G:H4'	2.43	0.49
1:A:1557:G:H2'	1:A:1558:C:O4'	2.12	0.49
1:A:2566:U:H2'	1:A:2567:C:C6	2.47	0.49
23:W:33:ASP:N	23:W:33:ASP:OD1	2.45	0.49
24:Y:66:PRO:C	24:Y:68:GLY:N	2.70	0.49
1:A:2376:C:O2'	1:A:2377:U:O4'	2.25	0.49
2:B:17:A:H2'	2:B:18:A:H8	1.77	0.49
23:W:124:THR:O	23:W:127:ARG:HB3	2.12	0.49
1:A:202:A:H1'	1:A:2462:A:C6	2.48	0.49
1:A:317:G:O2'	1:A:318:A:OP1	2.30	0.49
1:A:1096:A:N3	1:A:2780:G:O2'	2.43	0.49
18:R:2:LYS:O	18:R:6:ILE:HG12	2.12	0.49
19:S:17:GLU:OE1	19:S:20:ARG:NH2	2.46	0.49
6:F:59:GLN:CD	6:F:60:LYS:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:31:PRO:HB3	20:T:50:ASN:H	1.78	0.49
1:A:2659:G:H2'	1:A:2660:G:H8	1.77	0.49
1:A:200:A:OP2	1:A:2459:A:O2'	2.31	0.49
1:A:307:A:C5	1:A:308:C:C4	3.01	0.49
1:A:674:G:H4'	1:A:697:G:H4'	1.94	0.49
1:A:1712:G:O2'	1:A:2020:U:O4	2.27	0.49
1:A:2794:A:OP2	1:A:2795:G:N2	2.44	0.49
2:B:16:G:H2'	2:B:17:A:C8	2.48	0.49
6:F:76:MET:O	6:F:80:VAL:N	2.42	0.49
20:T:27:MET:SD	20:T:36:MET:SD	3.11	0.49
1:A:306:C:N4	1:A:307:A:H62	2.11	0.49
1:A:1520:A:N6	1:A:1564:C:H42	2.04	0.49
1:A:1425:C:H2'	1:A:1426:A:H8	1.77	0.48
12:L:95:LEU:HD12	13:M:4:ILE:HD13	1.95	0.48
1:A:674:G:H2'	1:A:675:C:H6	1.78	0.48
1:A:868:A:H5"	1:A:869:U:C6	2.48	0.48
1:A:1855:C:OP1	3:C:223:SER:OG	2.31	0.48
1:A:2096:G:H2'	1:A:2098:G:H8	1.77	0.48
1:A:2254:A:H1'	1:A:2255:C:OP2	2.13	0.48
1:A:2655:C:H2'	1:A:2656:G:H8	1.78	0.48
1:A:89:U:H5'	1:A:90:A:OP2	2.13	0.48
1:A:407:A:C2	1:A:408:G:H1'	2.48	0.48
1:A:767:U:C4	1:A:768:G:C5	3.01	0.48
1:A:1578:G:H1'	1:A:1588:A:H62	1.77	0.48
1:A:2106:A:H2'	1:A:2107:C:C6	2.47	0.48
1:A:2207:C:O4'	24:Y:47:ARG:CB	2.62	0.48
1:A:2319:G:O2'	1:A:2375:A:OP2	2.18	0.48
9:I:79:LEU:HB2	9:I:113:GLY:HA2	1.96	0.48
15:O:52:ASP:HB3	15:O:84:THR:HG22	1.95	0.48
1:A:1100:A:H2'	1:A:1151:U:H3	1.79	0.48
2:B:74:G:C6	2:B:99:A:N1	2.81	0.48
2:B:107:G:H2'	2:B:108:C:C6	2.48	0.48
17:Q:35:ASP:OD2	17:Q:36:GLY:N	2.46	0.48
20:T:35:GLU:OE1	20:T:45:ALA:N	2.46	0.48
23:W:379:ARG:O	23:W:381:LYS:NZ	2.46	0.48
24:Y:67:ASN:HD21	24:Y:187:GLU:CB	2.17	0.48
1:A:297:G:H4'	1:A:304:G:O2'	2.13	0.48
1:A:419:G:N2	1:A:448:A:OP2	2.40	0.48
1:A:1504:A:H4'	1:A:1505:U:O4'	2.14	0.48
23:W:85:VAL:HG21	23:W:159:VAL:HG13	1.94	0.48
1:A:2110:C:O2'	1:A:2111:A:H5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2522:U:O2'	23:W:433:ARG:NH1	2.47	0.48
1:A:2560:A:H61	1:A:2691:A:H61	1.62	0.48
6:F:86:ARG:HG3	6:F:142:VAL:HG13	1.95	0.48
9:I:35:HIS:O	9:I:35:HIS:ND1	2.47	0.48
1:A:351:G:N2	1:A:354:A:OP2	2.44	0.48
1:A:580:U:H2'	1:A:581:C:C6	2.48	0.48
1:A:897:G:H2'	1:A:898:U:C6	2.48	0.48
1:A:1518:G:N2	1:A:1566:G:H22	2.11	0.48
1:A:2131:U:H2'	1:A:2132:A:H8	1.77	0.48
23:W:87:ILE:HD11	23:W:155:LEU:HD21	1.95	0.48
23:W:338:THR:C	23:W:341:PRO:HD2	2.39	0.48
1:A:202:A:C2	1:A:2462:A:H2'	2.49	0.48
1:A:304:G:H2'	1:A:305:A:H8	1.79	0.48
1:A:580:U:H5'	12:L:42:SER:HB2	1.96	0.48
1:A:1556:A:H3'	1:A:1557:G:H8	1.77	0.48
1:A:2572:G:H2'	1:A:2573:G:C8	2.49	0.48
12:L:97:ASP:C	12:L:97:ASP:OD1	2.57	0.48
23:W:184:PRO:HD3	23:W:233:MET:O	2.13	0.48
1:A:2619:A:H5'	1:A:2620:C:OP2	2.13	0.48
1:A:2911:G:H2'	1:A:2912:A:C8	2.49	0.48
12:L:50:ARG:O	12:L:54:LYS:NZ	2.47	0.48
16:P:40:MET:HE3	16:P:40:MET:HA	1.95	0.48
1:A:306:C:H2'	1:A:307:A:C8	2.49	0.48
1:A:2353:U:H2'	1:A:2414:C:C5	2.49	0.48
8:H:112:MET:HE3	8:H:112:MET:HA	1.95	0.48
1:A:275:A:N6	1:A:297:G:H1'	2.29	0.47
1:A:1015:G:H2'	1:A:1016:U:C6	2.48	0.47
1:A:1476:C:H2'	1:A:1477:A:H8	1.79	0.47
1:A:912:C:H5"	1:A:913:A:N7	2.29	0.47
1:A:2352:G:H2'	1:A:2353:U:C6	2.49	0.47
2:B:12:U:H3	2:B:105:A:H5'	1.78	0.47
2:B:17:A:H2'	2:B:18:A:C8	2.48	0.47
18:R:10:THR:O	18:R:14:ILE:HG13	2.13	0.47
22:V:131:VAL:O	22:V:133:LYS:N	2.42	0.47
1:A:424:G:O6	1:A:444:U:C2	2.66	0.47
1:A:2373:U:O2'	1:A:2375:A:H3'	2.13	0.47
15:O:89:GLU:HA	15:O:89:GLU:OE1	2.15	0.47
23:W:240:TYR:CD2	23:W:240:TYR:O	2.67	0.47
24:Y:201:PRO:HG2	24:Y:208:TYR:CE1	2.44	0.47
1:A:807:G:H2'	1:A:808:A:O4'	2.14	0.47
1:A:1656:C:O2'	1:A:1657:C:H6	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2125:U:H2'	1:A:2126:G:C8	2.43	0.47
1:A:2197:G:H2'	1:A:2198:G:H21	1.78	0.47
1:A:1046:A:H2'	1:A:1047:A:C8	2.49	0.47
1:A:1494:G:H2'	1:A:1495:C:O4'	2.15	0.47
1:A:2412:G:N3	1:A:2412:G:H2'	2.30	0.47
23:W:97:THR:CG2	24:Y:55:ASN:CG	2.76	0.47
1:A:352:G:N2	1:A:524:A:N7	2.62	0.47
1:A:662:U:H2'	1:A:663:G:H8	1.78	0.47
1:A:1553:A:H3'	1:A:1554:U:C6	2.50	0.47
1:A:1819:C:O2'	3:C:208:ALA:HB2	2.15	0.47
1:A:2379:C:H2'	1:A:2380:G:O4'	2.14	0.47
1:A:2889:A:H2'	1:A:2890:U:C6	2.50	0.47
2:B:7:G:O2'	2:B:8:G:OP1	2.29	0.47
2:B:12:U:C2	2:B:105:A:H8	2.33	0.47
2:B:74:G:O6	2:B:99:A:N1	2.48	0.47
18:R:54:LYS:O	18:R:57:ILE:HG12	2.14	0.47
22:V:48:LEU:HD21	22:V:53:ARG:HD3	1.96	0.47
22:V:69:GLN:HE22	22:V:73:GLU:CD	2.23	0.47
24:Y:59:ILE:HD13	24:Y:201:PRO:HG3	1.94	0.47
24:Y:104:ILE:HG12	24:Y:108:TRP:CD1	2.50	0.47
24:Y:118:PRO:HG3	24:Y:145:VAL:HG12	1.97	0.47
1:A:805:G:H21	1:A:2010:A:N6	2.13	0.47
1:A:829:A:N1	3:C:225:MET:HE3	2.30	0.47
1:A:1218:U:H2'	1:A:1220:G:N3	2.30	0.47
1:A:2385:C:H2'	1:A:2390:A:N1	2.30	0.47
1:A:2409:U:HO2'	1:A:2410:C:P	2.38	0.47
1:A:200:A:H61	1:A:2274:U:H5'	1.80	0.47
1:A:315:C:H4'	1:A:316:G:O4'	2.14	0.47
1:A:579:G:H2'	1:A:580:U:C6	2.50	0.47
1:A:1306:G:O5'	14:N:15:ARG:NH2	2.48	0.47
1:A:1552:C:H2'	1:A:1553:A:C8	2.50	0.47
1:A:2780:G:H3'	1:A:2781:C:C6	2.48	0.47
1:A:675:C:H1'	1:A:685:U:H3	1.79	0.47
1:A:687:U:H3'	1:A:688:G:H8	1.78	0.47
1:A:696:C:H2'	1:A:697:G:H5'	1.97	0.47
1:A:1096:A:C2'	1:A:1097:A:H4'	2.40	0.47
1:A:1244:A:C8	9:I:4:HIS:HB3	2.50	0.47
1:A:2697:G:H1'	6:F:113:PRO:HD2	1.95	0.47
1:A:2831:A:H2'	1:A:2832:G:C8	2.50	0.47
2:B:35:C:N4	2:B:46:A:O2'	2.47	0.47
22:V:64:ASP:HB3	22:V:67:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:132:ASP:CG	24:Y:139:ASN:ND2	2.73	0.47
1:A:759:G:H3'	1:A:760:G:C8	2.50	0.46
1:A:1556:A:H2'	1:A:1557:G:C8	2.50	0.46
1:A:2234:C:H2'	1:A:2235:G:H8	1.80	0.46
1:A:2321:U:H2'	1:A:2322:C:H6	1.79	0.46
11:K:32:HIS:NE2	11:K:88:GLU:OE1	2.47	0.46
24:Y:117:THR:C	24:Y:121:MET:SD	2.98	0.46
1:A:63:G:H8	1:A:63:G:P	2.37	0.46
1:A:377:G:O2'	1:A:378:C:OP1	2.28	0.46
1:A:1079:U:O2'	1:A:1080:G:H5"	2.15	0.46
2:B:100:G:C2	2:B:101:U:C4	3.03	0.46
6:F:104:LEU:HD13	6:F:116:ILE:HB	1.97	0.46
6:F:149:ILE:H	6:F:149:ILE:CD1	2.28	0.46
1:A:198:A:H2'	1:A:253:G:H21	1.80	0.46
1:A:465:U:H2'	1:A:466:C:H6	1.79	0.46
1:A:1098:C:N3	1:A:1154:U:C4	2.84	0.46
1:A:1214:U:H2'	1:A:1215:U:C5	2.49	0.46
1:A:1696:G:O2'	1:A:1697:A:H8	1.97	0.46
1:A:2107:C:O2'	1:A:2462:A:N3	2.49	0.46
1:A:2111:A:H2'	1:A:2112:G:C8	2.50	0.46
1:A:2122:G:C2	1:A:2254:A:C5	3.03	0.46
9:I:102:ILE:HD12	9:I:109:VAL:HB	1.98	0.46
1:A:201:C:H5	1:A:251:G:H1	1.63	0.46
1:A:305:A:C8	1:A:306:C:C5	3.04	0.46
1:A:970:A:H2'	1:A:971:A:C8	2.50	0.46
1:A:1445:A:H2'	1:A:1446:C:H6	1.80	0.46
1:A:2454:A:H5'	1:A:2456:C:O4'	2.15	0.46
1:A:2567:C:H2'	1:A:2568:C:O2	2.15	0.46
17:Q:33:ARG:HA	17:Q:33:ARG:NE	2.30	0.46
19:S:8:LEU:HB2	19:S:28:LEU:HD13	1.97	0.46
1:A:279:A:H2'	1:A:280:G:H8	1.79	0.46
1:A:1244:A:O2'	1:A:1245:G:O5'	2.34	0.46
1:A:2149:G:C2	1:A:2150:G:C5	3.04	0.46
1:A:2401:G:H21	1:A:2402:A:N6	2.12	0.46
23:W:189:SER:OG	25:W:501:GNP:O1G	2.30	0.46
1:A:296:G:HO2'	1:A:297:G:P	2.36	0.46
2:B:78:U:O4	2:B:94:G:O6	2.34	0.46
17:Q:76:LYS:CG	17:Q:90:TYR:HB3	2.37	0.46
1:A:2313:C:H1'	1:A:2354:G:N2	2.30	0.46
1:A:690:A:N1	1:A:2398:A:H4'	2.31	0.46
1:A:1343:C:O2'	1:A:1344:C:O5'	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2828:G:H2'	1:A:2829:G:C8	2.51	0.46
9:I:79:LEU:HB3	9:I:115:GLY:H	1.80	0.46
23:W:18:THR:OG1	25:W:502:GNP:O1A	2.30	0.46
23:W:265:LEU:HB2	23:W:293:VAL:HG12	1.98	0.46
24:Y:64:VAL:HG12	24:Y:155:GLU:HB2	1.97	0.46
1:A:878:G:H2'	1:A:879:G:C8	2.51	0.46
1:A:905:G:C4	1:A:2297:A:H2'	2.51	0.46
1:A:1071:G:N7	1:A:1181:C:H1'	2.31	0.46
1:A:2358:A:H3'	1:A:2359:G:H8	1.81	0.46
1:A:2425:G:N2	1:A:2426:G:N7	2.64	0.46
1:A:2426:G:C5	1:A:2427:U:C4	3.04	0.46
9:I:69:ILE:HD12	9:I:70:ASN:H	1.80	0.46
18:R:1:MET:HA	18:R:4:ASN:ND2	2.31	0.46
1:A:153:C:H1'	1:A:177:G:N2	2.30	0.46
1:A:332:G:H2'	1:A:333:A:H8	1.81	0.46
1:A:416:U:O4'	1:A:417:G:N2	2.48	0.46
1:A:630:A:N1	1:A:856:G:O2'	2.46	0.46
1:A:677:A:O2'	1:A:678:A:OP1	2.32	0.46
1:A:698:C:H3'	1:A:699:A:H8	1.81	0.46
1:A:1559:C:H2'	1:A:1560:U:H6	1.81	0.46
22:V:125:ILE:HD13	22:V:137:ILE:HD11	1.98	0.46
22:V:159:GLN:N	22:V:171:ASP:OD1	2.49	0.46
1:A:1002:G:O2'	1:A:1005:A:N6	2.40	0.45
1:A:2317:A:OP1	1:A:2368:G:H5"	2.15	0.45
1:A:2778:A:H5"	1:A:2779:A:H2'	1.97	0.45
1:A:2825:C:H5"	1:A:2826:A:N7	2.32	0.45
1:A:567:U:H2'	1:A:568:G:C8	2.51	0.45
1:A:1334:C:H2'	1:A:1335:A:H8	1.80	0.45
1:A:1396:C:H2'	1:A:1397:G:O4'	2.16	0.45
1:A:1445:A:H2'	1:A:1446:C:C6	2.52	0.45
1:A:1681:U:O2'	1:A:1789:A:N3	2.41	0.45
1:A:2647:G:N2	4:D:146:MET:HE1	2.32	0.45
2:B:34:C:H6	2:B:35:C:H5	1.64	0.45
5:E:120:ASP:OD1	5:E:120:ASP:N	2.46	0.45
6:F:88:LEU:HB2	6:F:132:VAL:HB	1.98	0.45
1:A:575:A:N3	1:A:576:G:N2	2.64	0.45
1:A:638:U:H2'	1:A:639:C:H6	1.81	0.45
1:A:744:C:H2'	1:A:745:C:C6	2.52	0.45
1:A:1343:C:HO2'	1:A:1344:C:C5'	2.30	0.45
1:A:2264:G:H2'	1:A:2265:U:O4'	2.17	0.45
1:A:2321:U:O2'	1:A:2322:C:OP1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2440:A:C6	1:A:2441:A:H1'	2.51	0.45
1:A:2576:U:H5'	1:A:2595:A:C2	2.52	0.45
1:A:2727:U:H2'	1:A:2728:U:C6	2.52	0.45
23:W:296:TRP:HH2	23:W:306:MET:SD	2.39	0.45
1:A:852:G:H21	1:A:878:G:H1'	1.81	0.45
1:A:1150:C:H3'	1:A:1151:U:H5"	1.97	0.45
1:A:1438:C:HO2'	1:A:1439:U:P	2.39	0.45
1:A:1696:G:C4	1:A:1697:A:C8	3.05	0.45
1:A:1846:G:HO2'	1:A:1847:U:P	2.38	0.45
1:A:2376:C:O2'	1:A:2377:U:O5'	2.34	0.45
2:B:63:C:N4	2:B:107:G:OP2	2.33	0.45
1:A:688:G:H1'	1:A:691:U:OP1	2.17	0.45
1:A:759:G:C6	1:A:760:G:C6	3.04	0.45
1:A:2127:U:H2'	1:A:2128:U:O4'	2.17	0.45
1:A:2355:U:OP2	1:A:2356:A:O2'	2.33	0.45
1:A:2875:A:N7	1:A:2893:A:O2'	2.35	0.45
23:W:158:ALA:O	23:W:161:GLU:HG2	2.16	0.45
1:A:304:G:N7	1:A:411:G:N2	2.65	0.45
1:A:415:C:H5"	1:A:416:U:OP1	2.16	0.45
1:A:767:U:H2'	1:A:768:G:O4'	2.17	0.45
1:A:1216:C:H2'	1:A:1217:U:H5'	1.99	0.45
1:A:1684:U:H2'	1:A:1685:A:H5"	1.98	0.45
1:A:1832:A:H2	1:A:1852:G:H1'	1.82	0.45
20:T:27:MET:HE3	20:T:27:MET:C	2.42	0.45
1:A:1559:C:H2'	1:A:1560:U:C6	2.52	0.45
1:A:280:G:C6	1:A:281:A:C6	3.05	0.45
1:A:332:G:H2'	1:A:333:A:C8	2.51	0.45
1:A:414:C:HO2'	1:A:415:C:P	2.40	0.45
1:A:1550:C:H2'	1:A:1551:C:C6	2.52	0.45
1:A:2059:A:H5'	1:A:2060:A:OP1	2.16	0.45
1:A:2819:A:H4'	1:A:2820:U:H5"	1.99	0.45
6:F:28:LYS:HG2	6:F:29:GLY:H	1.82	0.45
15:O:91:GLU:O	15:O:91:GLU:CD	2.59	0.45
1:A:428:A:H3'	1:A:434:U:O4	2.17	0.45
1:A:675:C:C2	1:A:676:G:C8	3.05	0.45
1:A:1094:A:C8	1:A:1157:A:C6	3.05	0.45
1:A:1345:U:O2'	1:A:1346:A:O5'	2.32	0.45
1:A:1619:A:H2'	1:A:1620:A:C8	2.52	0.45
1:A:1696:G:H5"	10:J:35:THR:OG1	2.17	0.45
1:A:2625:U:O2'	1:A:2626:G:N7	2.50	0.45
1:A:2820:U:H2'	1:A:2821:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:224:ARG:HG3	22:V:225:TYR:H	1.81	0.45
1:A:305:A:N6	1:A:411:G:H21	2.13	0.45
1:A:689:A:H5"	1:A:690:A:OP2	2.17	0.45
1:A:1862:C:N3	1:A:1863:U:O2'	2.43	0.45
1:A:2291:U:C2	1:A:2308:G:N7	2.85	0.45
1:A:2374:G:O6	1:A:2400:G:C6	2.70	0.45
1:A:2398:A:O2'	1:A:2399:G:OP1	2.33	0.45
1:A:2555:G:H5'	1:A:2556:C:OP2	2.17	0.45
1:A:2655:C:H2'	1:A:2656:G:C8	2.52	0.45
1:A:2694:A:H3'	1:A:2695:C:C6	2.52	0.45
1:A:302:A:OP1	1:A:302:A:H3'	2.17	0.44
1:A:303:G:HO2'	1:A:304:G:P	2.41	0.44
1:A:327:G:H2'	1:A:328:G:C8	2.52	0.44
1:A:679:A:C5	1:A:680:G:H1'	2.52	0.44
1:A:1011:C:H2'	1:A:1012:G:H8	1.82	0.44
1:A:1579:A:H3'	1:A:1580:A:C8	2.52	0.44
1:A:2018:A:H2'	1:A:2019:C:O4'	2.17	0.44
23:W:361:ASP:HA	23:W:364:MET:HE1	1.99	0.44
1:A:90:A:H61	1:A:503:C:H41	1.64	0.44
1:A:2010:A:N3	1:A:2010:A:H2'	2.32	0.44
16:P:88:GLY:O	16:P:89:LYS:HD2	2.17	0.44
1:A:287:G:N1	1:A:289:C:OP1	2.51	0.44
1:A:1244:A:H8	9:I:4:HIS:HB3	1.81	0.44
1:A:1513:U:H3	1:A:1572:G:H1	1.66	0.44
1:A:2309:G:H4'	1:A:2356:A:OP1	2.18	0.44
1:A:2442:G:H2'	1:A:2443:G:O4'	2.17	0.44
5:E:103:LYS:HA	5:E:106:ARG:HE	1.83	0.44
1:A:49:A:H2	1:A:119:U:H3	1.65	0.44
1:A:202:A:H1'	1:A:2462:A:C5	2.53	0.44
1:A:776:G:O2'	1:A:810:G:H4'	2.17	0.44
1:A:1080:G:C5	1:A:1168:G:C2	3.06	0.44
1:A:1425:C:H2'	1:A:1426:A:C8	2.53	0.44
1:A:2543:U:H2'	1:A:2544:C:C6	2.52	0.44
1:A:2917:G:OP2	1:A:2917:G:N2	2.33	0.44
22:V:230:ILE:O	22:V:230:ILE:HG13	2.16	0.44
22:V:261:GLU:O	22:V:265:ARG:N	2.51	0.44
23:W:322:TYR:HB2	23:W:425:GLY:H	1.82	0.44
23:W:340:MET:O	23:W:344:ILE:HG12	2.17	0.44
3:C:68:LYS:HB3	3:C:70:ASP:OD1	2.17	0.44
4:D:121:GLY:HA2	4:D:161:PRO:HB3	1.98	0.44
4:D:146:MET:HE2	4:D:146:MET:HB3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:C:N3	1:A:406:G:H2'	2.32	0.44
1:A:760:G:H2'	1:A:761:U:C6	2.53	0.44
1:A:2147:U:OP2	1:A:2147:U:H3'	2.18	0.44
1:A:2204:U:H2'	1:A:2205:A:O4'	2.16	0.44
1:A:2291:U:H4'	1:A:2357:A:N3	2.32	0.44
1:A:2311:G:OP2	1:A:2311:G:H8	2.01	0.44
1:A:2320:U:O4	1:A:2370:G:O6	2.34	0.44
1:A:2439:G:H2'	1:A:2440:A:C8	2.52	0.44
2:B:64:A:H5"	2:B:106:C:N3	2.31	0.44
3:C:125:LYS:HE2	3:C:125:LYS:HB3	1.88	0.44
6:F:30:PRO:HD2	6:F:80:VAL:HG12	1.99	0.44
9:I:96:LEU:HB2	9:I:102:ILE:CG2	2.47	0.44
10:J:20:LEU:HB3	10:J:40:LEU:HD11	1.98	0.44
10:J:114:MET:HE3	10:J:114:MET:HB3	1.87	0.44
24:Y:194:ASP:O	24:Y:198:LYS:HB2	2.17	0.44
1:A:202:A:H1'	1:A:2462:A:N6	2.32	0.44
1:A:2293:C:H2'	1:A:2294:U:C6	2.53	0.44
8:H:90:ASP:C	8:H:90:ASP:OD1	2.61	0.44
1:A:430:C:H42	1:A:437:A:H62	1.65	0.44
1:A:624:C:H2'	1:A:625:C:C6	2.53	0.44
1:A:2254:A:H4'	1:A:2255:C:O5'	2.18	0.44
1:A:2492:C:H2'	1:A:2493:C:C6	2.52	0.44
1:A:2682:U:H3'	1:A:2683:A:C8	2.53	0.44
1:A:2778:A:OP1	6:F:4:VAL:N	2.51	0.44
1:A:2823:C:H3'	1:A:2824:G:C8	2.47	0.44
6:F:139:LYS:HA	6:F:142:VAL:HG12	1.99	0.44
9:I:79:LEU:HB3	9:I:115:GLY:N	2.32	0.44
17:Q:73:GLY:HA3	17:Q:91:PRO:HA	1.99	0.44
18:R:10:THR:HG23	18:R:11:THR:H	1.83	0.44
23:W:380:LEU:HD12	23:W:381:LYS:H	1.82	0.44
1:A:455:G:H2'	1:A:456:A:C8	2.53	0.44
1:A:904:A:H2'	1:A:905:G:C6	2.53	0.44
1:A:2326:C:C4	1:A:2348:C:H4'	2.52	0.44
1:A:2605:G:N3	1:A:2605:G:H2'	2.33	0.44
2:B:47:C:O2'	2:B:48:G:OP1	2.33	0.44
6:F:45:LYS:HB2	6:F:53:VAL:HA	2.00	0.44
11:K:91:ARG:HG2	11:K:115:GLU:OE1	2.18	0.44
14:N:14:PRO:C	14:N:16:LYS:H	2.26	0.44
17:Q:45:LEU:HD11	17:Q:69:ALA:HB2	1.99	0.44
22:V:41:ASN:HB3	22:V:44:ILE:HG22	1.99	0.44
22:V:222:LYS:HB3	22:V:222:LYS:HE3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:273:GLY:O	22:V:275:LEU:HD23	2.18	0.44
1:A:1011:C:H2'	1:A:1012:G:C8	2.52	0.43
1:A:1343:C:H41	1:A:1652:C:N4	2.15	0.43
1:A:2786:A:N3	1:A:2786:A:H2'	2.32	0.43
6:F:108:VAL:HA	6:F:153:ARG:CZ	2.47	0.43
17:Q:49:ARG:NH1	17:Q:64:ASP:OD2	2.51	0.43
24:Y:58:GLN:OE1	24:Y:60:ARG:HB3	2.18	0.43
1:A:78:U:H2'	1:A:79:C:H6	1.83	0.43
1:A:150:A:H61	1:A:179:A:H2	1.65	0.43
1:A:151:U:H2'	1:A:152:C:H6	1.83	0.43
1:A:340:U:H2'	1:A:341:G:O4'	2.18	0.43
1:A:879:G:H2'	1:A:880:C:C6	2.53	0.43
1:A:1460:G:HO2'	1:A:1461:A:H8	1.62	0.43
1:A:1551:C:H2'	1:A:1552:C:O4'	2.18	0.43
1:A:1759:U:H5	1:A:1773:G:C4	2.36	0.43
1:A:2129:G:H2'	1:A:2130:G:H8	1.82	0.43
1:A:2310:C:H1'	1:A:2417:A:N7	2.32	0.43
12:L:61:TRP:CZ2	12:L:94:MET:HB2	2.53	0.43
23:W:297:ASP:OD2	25:W:501:GNP:N2	2.43	0.43
23:W:350:HIS:CE1	23:W:391:LYS:CB	3.02	0.43
1:A:316:G:O2'	1:A:317:G:H5'	2.18	0.43
1:A:331:C:H2'	1:A:332:G:H8	1.82	0.43
1:A:662:U:H2'	1:A:663:G:C8	2.53	0.43
1:A:2092:C:H5"	1:A:2468:A:N6	2.33	0.43
1:A:2122:G:N1	1:A:2254:A:N7	2.66	0.43
1:A:2421:A:H2'	1:A:2422:U:H5'	1.99	0.43
1:A:2672:G:H2'	1:A:2673:A:H8	1.83	0.43
1:A:2829:G:H2'	1:A:2830:A:C8	2.54	0.43
15:O:56:ILE:HD13	15:O:77:ARG:HH21	1.83	0.43
1:A:607:G:N2	12:L:37:GLN:OE1	2.39	0.43
1:A:2669:G:OP1	7:G:100:LYS:NZ	2.48	0.43
9:I:83:ASN:HA	9:I:117:LEU:HD13	1.99	0.43
18:R:38:GLU:HG2	18:R:39:ASN:N	2.33	0.43
22:V:213:LEU:HB3	22:V:221:LEU:HG	1.99	0.43
23:W:26:GLU:C	23:W:27:ARG:HD3	2.43	0.43
1:A:339:A:H2'	1:A:340:U:C6	2.54	0.43
1:A:462:A:C6	1:A:2438:G:N1	2.86	0.43
1:A:1552:C:O2'	1:A:1553:A:H5'	2.18	0.43
2:B:79:C:N3	2:B:93:U:O4	2.51	0.43
10:J:102:MET:HE2	10:J:102:MET:HB3	1.87	0.43
22:V:144:ASN:O	22:V:144:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:G:H2'	1:A:313:U:O4'	2.18	0.43
1:A:1528:U:H4'	1:A:1529:G:H5'	1.99	0.43
1:A:1556:A:C3'	1:A:1557:G:H8	2.32	0.43
6:F:69:THR:OG1	6:F:70:ARG:N	2.52	0.43
6:F:88:LEU:HD23	6:F:88:LEU:HA	1.83	0.43
23:W:132:ASP:OD2	24:Y:139:ASN:ND2	2.51	0.43
1:A:327:G:N2	1:A:400:U:O2	2.44	0.43
1:A:902:G:C2	1:A:903:G:H1'	2.53	0.43
1:A:1572:G:H8	1:A:1572:G:OP2	2.02	0.43
1:A:2206:C:H2'	1:A:2207:C:C6	2.54	0.43
1:A:2465:G:H8	1:A:2465:G:O5'	2.02	0.43
1:A:2560:A:H1'	6:F:158:TYR:CE2	2.54	0.43
2:B:37:A:H1'	2:B:45:C:H2'	2.00	0.43
6:F:48:ASP:OD1	6:F:49:ASN:N	2.52	0.43
23:W:189:SER:H	25:W:501:GNP:HNB3	1.67	0.43
23:W:414:GLU:OE2	23:W:418:ARG:NH2	2.36	0.43
24:Y:200:LYS:HD2	24:Y:200:LYS:HA	1.71	0.43
1:A:1173:A:O2'	1:A:1174:A:OP1	2.31	0.43
1:A:2193:C:H3'	1:A:2194:G:C8	2.54	0.43
1:A:2429:G:O2'	1:A:2430:U:O4'	2.34	0.43
1:A:2431:U:O2'	1:A:2432:C:H3'	2.19	0.43
1:A:2433:C:O2	1:A:2443:G:N1	2.51	0.43
6:F:89:GLU:C	6:F:90:LEU:HD12	2.44	0.43
1:A:283:G:C2	1:A:288:C:O2	2.72	0.43
1:A:822:G:OP1	1:A:824:G:O2'	2.37	0.43
1:A:1571:G:C2'	1:A:1572:G:H5'	2.49	0.43
1:A:2103:U:O2'	1:A:2626:G:H1'	2.19	0.43
1:A:2119:A:C6	1:A:2259:G:O6	2.72	0.43
1:A:2414:C:O2'	17:Q:49:ARG:NH1	2.41	0.43
1:A:2432:C:H2'	1:A:2443:G:H1	1.84	0.43
8:H:9:LYS:NZ	8:H:9:LYS:HB2	2.34	0.43
11:K:36:VAL:HA	11:K:40:ARG:O	2.19	0.43
1:A:259:A:H2'	1:A:260:A:C8	2.52	0.43
1:A:294:G:C6	1:A:295:G:N7	2.87	0.43
1:A:1177:G:N2	1:A:1178:U:O4	2.45	0.43
1:A:1734:A:H2'	1:A:1735:A:C8	2.54	0.43
1:A:2428:G:N3	1:A:2428:G:H2'	2.34	0.43
1:A:2670:A:H2'	1:A:2671:G:H8	1.83	0.43
2:B:52:G:H3'	2:B:53:U:C6	2.54	0.43
22:V:198:SER:C	22:V:199:ILE:HD13	2.44	0.43
1:A:421:A:H62	1:A:447:G:H21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:A:C6	1:A:698:C:H1'	2.54	0.42
1:A:1166:G:H2'	1:A:1167:C:C6	2.54	0.42
1:A:1394:G:H2'	1:A:1395:C:C6	2.54	0.42
1:A:2131:U:C2	1:A:2132:A:C8	3.07	0.42
1:A:2321:U:HO2'	1:A:2322:C:P	2.41	0.42
2:B:24:C:H2'	2:B:25:A:O4'	2.19	0.42
3:C:205:ILE:HG23	3:C:210:ARG:HB3	2.00	0.42
12:L:74:LEU:HD11	12:L:114:LYS:HG3	2.00	0.42
17:Q:35:ASP:HA	17:Q:75:VAL:HB	2.00	0.42
23:W:32:GLU:O	23:W:32:GLU:HG2	2.19	0.42
1:A:194:A:H2'	1:A:195:C:C6	2.54	0.42
1:A:2137:U:H2'	1:A:2138:U:C6	2.54	0.42
1:A:2443:G:H2'	1:A:2444:G:H8	1.83	0.42
23:W:350:HIS:ND1	23:W:391:LYS:HB3	2.34	0.42
1:A:304:G:C4	1:A:305:A:C8	3.08	0.42
1:A:765:A:H2'	1:A:766:C:O4'	2.19	0.42
1:A:874:U:C2	1:A:2455:A:N6	2.88	0.42
1:A:1507:U:H2'	1:A:1508:C:C6	2.54	0.42
1:A:2318:G:H1'	1:A:2375:A:H62	1.83	0.42
1:A:2378:G:N2	1:A:2397:C:O2'	2.40	0.42
1:A:2494:C:O2'	1:A:2495:C:O4'	2.35	0.42
3:C:105:LEU:CD1	3:C:156:ARG:HB2	2.49	0.42
23:W:97:THR:CG2	24:Y:52:PRO:HD2	2.48	0.42
24:Y:194:ASP:HA	24:Y:197:LEU:CG	2.48	0.42
1:A:283:G:N1	1:A:288:C:N3	2.49	0.42
1:A:1515:C:H2'	1:A:1516:A:C8	2.54	0.42
1:A:2220:A:H2'	1:A:2221:C:O4'	2.20	0.42
1:A:2448:U:H2'	1:A:2449:C:C6	2.54	0.42
1:A:2716:U:H2'	1:A:2717:G:O4'	2.19	0.42
1:A:2775:U:H3'	1:A:2776:G:H8	1.84	0.42
22:V:200:ILE:HD11	22:V:202:LEU:HD13	2.02	0.42
24:Y:65:LEU:HD22	24:Y:65:LEU:HA	1.85	0.42
1:A:202:A:H5"	1:A:2272:U:H1'	2.00	0.42
1:A:430:C:H42	1:A:437:A:N6	2.18	0.42
1:A:488:U:O2'	5:E:46:GLN:OE1	2.26	0.42
1:A:873:U:H4'	1:A:2457:G:H2'	2.01	0.42
1:A:1075:A:H2'	1:A:1076:G:O4'	2.20	0.42
1:A:2327:A:N1	1:A:2347:G:H8	2.18	0.42
2:B:11:A:H2'	2:B:105:A:N6	2.35	0.42
22:V:23:LEU:O	22:V:122:ARG:NH1	2.44	0.42
24:Y:197:LEU:C	24:Y:199:ALA:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:G:H2'	1:A:298:U:C5	2.55	0.42
1:A:638:U:H2'	1:A:639:C:C6	2.54	0.42
1:A:873:U:O2	1:A:879:G:N2	2.52	0.42
1:A:1808:U:OP2	1:A:1813:A:N6	2.50	0.42
1:A:1819:C:H2'	1:A:1820:A:C8	2.55	0.42
1:A:1846:G:O2'	1:A:1847:U:OP1	2.32	0.42
1:A:2349:A:H2'	1:A:2362:A:N1	2.34	0.42
1:A:2423:C:C2	1:A:2424:C:H1'	2.55	0.42
1:A:2432:C:H1'	1:A:2444:G:N1	2.34	0.42
1:A:2686:A:H2'	1:A:2687:C:O4'	2.19	0.42
2:B:5:G:N3	2:B:5:G:H2'	2.34	0.42
18:R:2:LYS:HZ3	18:R:6:ILE:HG13	1.85	0.42
22:V:221:LEU:HD23	22:V:221:LEU:HA	1.87	0.42
1:A:254:A:O5'	1:A:254:A:H8	2.03	0.42
1:A:759:G:C2'	1:A:760:G:H5'	2.50	0.42
1:A:1253:A:H2'	1:A:1254:A:H8	1.84	0.42
1:A:2114:C:H42	1:A:2262:A:N6	2.17	0.42
1:A:2320:U:C4	1:A:2370:G:O6	2.73	0.42
1:A:2820:U:H2'	1:A:2821:U:H6	1.84	0.42
6:F:23:ASN:HB2	6:F:38:PHE:H	1.83	0.42
23:W:219:THR:HA	23:W:224:GLU:HA	2.01	0.42
1:A:90:A:N6	1:A:503:C:H41	2.17	0.42
1:A:418:A:H2	1:A:448:A:H5"	1.84	0.42
1:A:688:G:O2'	1:A:692:A:N7	2.50	0.42
1:A:868:A:H5"	1:A:869:U:H6	1.85	0.42
1:A:2439:G:H2'	1:A:2440:A:H8	1.85	0.42
2:B:53:U:O2'	2:B:54:U:OP1	2.36	0.42
24:Y:194:ASP:OD1	24:Y:197:LEU:HD21	2.20	0.42
1:A:75:G:H22	1:A:110:A:H2	1.67	0.42
1:A:1016:U:H2'	1:A:1017:C:C6	2.55	0.42
1:A:1080:G:H2'	1:A:1081:U:O4'	2.20	0.42
1:A:1303:U:H2'	1:A:1304:G:C8	2.55	0.42
1:A:2785:U:O2'	1:A:2786:A:OP2	2.35	0.42
6:F:55:ARG:HD2	6:F:57:SER:O	2.19	0.42
1:A:2559:U:O3'	1:A:2563:C:N4	2.53	0.42
5:E:68:LYS:HD3	5:E:68:LYS:HA	1.91	0.42
6:F:39:HIS:HD2	6:F:41:ASP:H	1.67	0.42
11:K:7:LEU:HD23	11:K:7:LEU:HA	1.88	0.42
22:V:138:ASN:HD21	22:V:146:ALA:HB3	1.84	0.42
23:W:391:LYS:HB2	23:W:391:LYS:HE3	1.40	0.42
1:A:66:C:C2	1:A:67:A:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1495:C:N4	1:A:1508:C:H42	2.17	0.41
1:A:1588:A:H3'	1:A:1589:G:H8	1.84	0.41
1:A:1617:A:H2'	1:A:1618:A:C8	2.55	0.41
1:A:2111:A:H2'	1:A:2112:G:H8	1.84	0.41
1:A:2143:A:O5'	1:A:2143:A:H8	2.03	0.41
1:A:2207:C:OP1	24:Y:211:ASN:CB	2.67	0.41
1:A:2209:U:H2'	1:A:2210:G:H8	1.85	0.41
23:W:132:ASP:N	24:Y:137:MET:CE	2.76	0.41
1:A:525:A:O2'	1:A:526:A:OP1	2.36	0.41
1:A:1210:A:H2'	1:A:1211:C:C6	2.54	0.41
1:A:1526:G:N2	1:A:1559:C:C2	2.88	0.41
1:A:2130:G:H2'	1:A:2131:U:H6	1.84	0.41
1:A:2153:G:OP1	24:Y:43:GLU:OE1	2.38	0.41
1:A:2373:U:C2	1:A:2375:A:H5'	2.55	0.41
1:A:2626:G:O2'	1:A:2627:A:O4'	2.23	0.41
1:A:2773:G:H2'	1:A:2774:C:C6	2.55	0.41
2:B:3:U:H4'	2:B:24:C:N3	2.36	0.41
3:C:105:LEU:HD11	3:C:156:ARG:HB2	2.02	0.41
9:I:89:THR:OG1	9:I:122:THR:O	2.33	0.41
17:Q:76:LYS:CG	17:Q:90:TYR:H	2.32	0.41
23:W:158:ALA:HA	23:W:161:GLU:OE1	2.20	0.41
1:A:222:A:N3	1:A:237:U:O2'	2.47	0.41
1:A:2291:U:C2	1:A:2292:C:C4	3.08	0.41
1:A:2559:U:H2'	6:F:175:GLY:HA2	2.02	0.41
2:B:3:U:O2'	2:B:25:A:H1'	2.20	0.41
9:I:93:PRO:O	9:I:97:LEU:CB	2.68	0.41
10:J:40:LEU:HD22	10:J:117:ILE:HD13	2.00	0.41
1:A:7:G:N2	1:A:2921:U:C2	2.89	0.41
1:A:697:G:N3	1:A:698:C:H5	2.18	0.41
1:A:1080:G:H8	1:A:1080:G:O5'	2.04	0.41
1:A:2119:A:H2'	1:A:2120:U:C6	2.56	0.41
1:A:2130:G:O6	1:A:2217:U:O4	2.37	0.41
1:A:2309:G:C2	1:A:2417:A:C2	3.09	0.41
1:A:2405:A:O2'	1:A:2406:A:P	2.78	0.41
1:A:2553:G:H22	1:A:2568:C:H5	1.69	0.41
1:A:2584:U:H6	1:A:2586:G:OP2	2.03	0.41
2:B:74:G:OP2	2:B:75:U:H5"	2.20	0.41
22:V:97:VAL:N	22:V:98:PRO:HD2	2.35	0.41
23:W:41:ARG:HA	23:W:57:ASP:O	2.21	0.41
24:Y:78:PHE:O	24:Y:120:MET:CE	2.68	0.41
1:A:284:C:H1'	1:A:288:C:O2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2216:A:C6	1:A:2217:U:C4	3.08	0.41
1:A:2317:A:OP2	1:A:2318:G:H8	2.03	0.41
1:A:2543:U:H2'	1:A:2544:C:H6	1.85	0.41
2:B:47:C:O2'	2:B:48:G:P	2.79	0.41
2:B:47:C:H2'	2:B:48:G:O4'	2.21	0.41
4:D:51:LEU:O	4:D:80:VAL:HA	2.20	0.41
6:F:85:GLU:C	6:F:86:ARG:HG2	2.46	0.41
22:V:217:TYR:HB3	22:V:220:ARG:HB2	2.02	0.41
23:W:124:THR:HA	23:W:127:ARG:NH1	2.35	0.41
24:Y:121:MET:HG3	24:Y:145:VAL:HG11	2.02	0.41
1:A:194:A:H2'	1:A:195:C:H6	1.83	0.41
1:A:677:A:H61	1:A:2432:C:H4'	1.86	0.41
1:A:1306:G:O2'	1:A:2041:G:O6	2.31	0.41
1:A:1831:A:H2'	1:A:1832:A:C8	2.56	0.41
1:A:2093:C:H2'	1:A:2094:C:H6	1.86	0.41
12:L:61:TRP:CH2	12:L:94:MET:HB2	2.55	0.41
23:W:21:ASN:ND2	23:W:30:ILE:HD11	2.33	0.41
23:W:55:LEU:HD12	23:W:55:LEU:HA	1.84	0.41
23:W:350:HIS:CE1	23:W:391:LYS:HB3	2.56	0.41
1:A:759:G:H2'	1:A:760:G:H5'	2.03	0.41
1:A:1220:G:O2'	1:A:1221:A:O5'	2.35	0.41
1:A:1632:G:H2'	1:A:1633:G:H8	1.85	0.41
1:A:1713:A:N3	1:A:1715:C:N4	2.69	0.41
1:A:2076:C:H2'	1:A:2077:G:H8	1.85	0.41
1:A:2644:U:H2'	1:A:2645:C:H6	1.84	0.41
4:D:47:GLU:HB3	4:D:88:MET:HG3	2.02	0.41
23:W:306:MET:O	23:W:310:GLU:HB2	2.20	0.41
1:A:305:A:C2'	1:A:306:C:H5'	2.49	0.41
1:A:420:U:O2'	1:A:470:A:N3	2.44	0.41
1:A:769:A:H2'	1:A:770:A:H8	1.86	0.41
1:A:908:A:H62	1:A:963:G:H21	1.67	0.41
1:A:2314:C:H6	1:A:2314:C:P	2.44	0.41
1:A:2326:C:C5	1:A:2348:C:H4'	2.56	0.41
1:A:2691:A:O5'	1:A:2691:A:H8	2.04	0.41
1:A:2785:U:O2'	1:A:2786:A:P	2.78	0.41
22:V:5:TRP:CD1	22:V:7:PRO:HD3	2.55	0.41
23:W:145:SER:O	23:W:149:GLY:N	2.50	0.41
23:W:393:PRO:HB2	23:W:395:PHE:CZ	2.56	0.41
1:A:230:A:H4'	1:A:231:A:O5'	2.20	0.41
1:A:331:C:H2'	1:A:332:G:C8	2.55	0.41
1:A:675:C:H1'	1:A:685:U:N3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:G:OP2	1:A:871:G:H2'	2.20	0.41
1:A:2095:C:H2'	1:A:2096:G:C8	2.55	0.41
1:A:2138:U:H2'	1:A:2139:G:H8	1.77	0.41
1:A:2140:U:O2'	1:A:2147:U:O2'	2.35	0.41
1:A:2228:A:N6	1:A:2254:A:C8	2.89	0.41
1:A:2316:A:H62	1:A:2375:A:N6	2.19	0.41
1:A:2321:U:O2'	1:A:2322:C:P	2.79	0.41
1:A:2569:C:H2'	1:A:2570:A:O4'	2.21	0.41
1:A:2674:G:H4'	1:A:2761:G:O2'	2.20	0.41
4:D:25:VAL:HG11	4:D:187:LEU:HD23	2.03	0.41
8:H:76:TYR:O	11:K:75:ARG:HG3	2.21	0.41
22:V:23:LEU:HD13	23:W:369:MET:HG2	2.03	0.41
23:W:41:ARG:HD3	23:W:75:GLN:O	2.20	0.41
1:A:276:C:O2'	1:A:306:C:O5'	2.37	0.41
1:A:278:A:N6	1:A:294:G:C6	2.88	0.41
1:A:681:C:H3'	1:A:682:G:H8	1.84	0.41
1:A:902:G:C6	1:A:970:A:N6	2.89	0.41
1:A:970:A:H1'	17:Q:34:ALA:HB1	2.03	0.41
1:A:1075:A:H3'	1:A:1076:G:C8	2.55	0.41
1:A:1279:C:H2'	1:A:1280:G:C8	2.56	0.41
1:A:1349:G:N2	1:A:1352:U:C4	2.89	0.41
1:A:2268:G:OP1	1:A:2268:G:H3'	2.20	0.41
1:A:2454:A:H4'	1:A:2455:A:H5"	2.03	0.41
2:B:11:A:H2'	2:B:105:A:C6	2.56	0.41
23:W:210:THR:HB	23:W:231:ALA:HA	2.02	0.41
1:A:303:G:H8	1:A:303:G:O5'	2.04	0.40
1:A:418:A:H4'	1:A:419:G:H4'	2.02	0.40
1:A:621:G:O2'	1:A:1294:A:OP1	2.38	0.40
1:A:1094:A:C8	1:A:1157:A:C5	3.09	0.40
1:A:1210:A:H2'	1:A:1211:C:H6	1.86	0.40
1:A:1527:C:C4	1:A:1528:U:O4	2.74	0.40
1:A:1555:A:O3'	1:A:1556:A:H8	2.05	0.40
2:B:16:G:H2'	2:B:17:A:H8	1.84	0.40
6:F:145:ILE:HD13	6:F:145:ILE:HA	1.92	0.40
8:H:93:PRO:HG3	8:H:114:ILE:HG13	2.03	0.40
9:I:93:PRO:HG3	9:I:105:LEU:HD22	2.03	0.40
14:N:21:MET:HE2	14:N:21:MET:HB2	1.83	0.40
24:Y:129:ARG:HG2	24:Y:129:ARG:O	2.21	0.40
1:A:268:A:N6	1:A:474:U:O2'	2.54	0.40
1:A:560:A:H2'	1:A:561:A:H8	1.86	0.40
1:A:766:C:H2'	1:A:767:U:H5"	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:A:C6	1:A:972:U:C2	3.09	0.40
1:A:1003:A:N6	1:A:2528:C:OP2	2.53	0.40
1:A:2029:G:C2	1:A:2030:A:C8	3.09	0.40
1:A:2111:A:H2'	1:A:2112:G:O4'	2.21	0.40
1:A:2318:G:O6	1:A:2369:A:H5"	2.21	0.40
1:A:2374:G:N2	1:A:2410:C:C2	2.87	0.40
1:A:2471:C:H2'	1:A:2472:C:C6	2.56	0.40
1:A:2779:A:H1'	1:A:2781:C:H41	1.86	0.40
1:A:2812:A:O2'	1:A:2813:U:OP1	2.36	0.40
2:B:18:A:H2'	2:B:19:G:C1'	2.52	0.40
2:B:28:C:H5"	2:B:29:C:C5	2.57	0.40
3:C:168:GLU:OE1	3:C:171:TYR:HB2	2.21	0.40
6:F:92:GLY:HA3	6:F:95:TYR:CD1	2.57	0.40
16:P:71:LEU:HD23	16:P:71:LEU:HA	1.88	0.40
23:W:283:HIS:ND1	23:W:322:TYR:OH	2.49	0.40
24:Y:202:ALA:O	24:Y:203:ALA:HB3	2.20	0.40
1:A:184:G:H4'	1:A:185:A:O5'	2.21	0.40
1:A:2122:G:O2'	1:A:2123:A:O4'	2.38	0.40
1:A:2351:A:HO2'	1:A:2352:G:P	2.41	0.40
1:A:2473:G:H2'	1:A:2474:G:C8	2.55	0.40
5:E:38:LEU:HD12	5:E:38:LEU:HA	1.91	0.40
9:I:10:GLU:HA	9:I:10:GLU:OE2	2.22	0.40
12:L:90:VAL:HG12	13:M:11:GLN:HE22	1.84	0.40
13:M:50:ASN:HB2	13:M:51:PRO:CD	2.48	0.40
1:A:93:C:H2'	1:A:94:A:C8	2.55	0.40
1:A:1000:G:H1'	1:A:2303:A:H2	1.86	0.40
1:A:1070:G:C5'	1:A:1071:G:H5"	2.51	0.40
1:A:1078:A:H2	1:A:1168:G:H22	1.69	0.40
1:A:1098:C:N3	1:A:1099:C:C4	2.90	0.40
1:A:1824:C:H2'	1:A:1825:U:C6	2.57	0.40
1:A:2054:C:H2'	1:A:2055:U:C6	2.57	0.40
1:A:2308:G:C5	1:A:2309:G:N7	2.89	0.40
1:A:2384:C:H2'	1:A:2385:C:O4'	2.22	0.40
11:K:18:THR:O	11:K:18:THR:OG1	2.32	0.40
14:N:14:PRO:O	14:N:15:ARG:HB3	2.22	0.40
23:W:15:GLY:HA2	25:W:502:GNP:PA	2.60	0.40
1:A:303:G:H2'	1:A:304:G:O4'	2.21	0.40
1:A:462:A:HO2'	1:A:463:U:P	2.43	0.40
1:A:1244:A:C4	1:A:1245:G:N2	2.90	0.40
1:A:1467:G:O2'	1:A:1540:A:N6	2.54	0.40
1:A:1576:G:C2	1:A:1577:C:C2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2312:C:C5	1:A:2418:G:C4	3.10	0.40
4:D:80:VAL:O	4:D:81:LYS:HD2	2.21	0.40
23:W:132:ASP:OD1	24:Y:137:MET:CE	2.70	0.40
23:W:325:ILE:HG22	23:W:327:PHE:CE1	2.57	0.40
24:Y:123:GLU:O	24:Y:127:ILE:HG22	2.21	0.40
24:Y:201:PRO:CG	24:Y:208:TYR:HE1	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	242/277 (87%)	234 (97%)	8 (3%)	0	100	100
4	D	205/209 (98%)	198 (97%)	7 (3%)	0	100	100
5	E	203/207 (98%)	194 (96%)	9 (4%)	0	100	100
6	F	173/179 (97%)	159 (92%)	14 (8%)	0	100	100
7	G	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
8	H	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
9	I	100/146 (68%)	94 (94%)	6 (6%)	0	100	100
10	J	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
11	K	111/115 (96%)	109 (98%)	2 (2%)	0	100	100
12	L	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
13	M	99/102 (97%)	93 (94%)	6 (6%)	0	100	100
14	N	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
15	O	90/95 (95%)	87 (97%)	3 (3%)	0	100	100
16	P	94/103 (91%)	89 (95%)	5 (5%)	0	100	100
17	Q	57/94 (61%)	51 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
19	S	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
20	T	52/59 (88%)	49 (94%)	3 (6%)	0	100	100
21	U	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
22	V	263/282 (93%)	252 (96%)	11 (4%)	0	100	100
23	W	409/436 (94%)	393 (96%)	16 (4%)	0	100	100
24	Y	168/232 (72%)	148 (88%)	17 (10%)	3 (2%)	7	29
All	All	3026/3323 (91%)	2876 (95%)	147 (5%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	Y	66	PRO
24	Y	67	ASN
24	Y	130	VAL

5.3.2 Protein sidechains (i)

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	
3	C	200/225 (89%)	200 (100%)	0	100	100
4	D	168/170 (99%)	168 (100%)	0	100	100
5	E	166/170 (98%)	166 (100%)	0	100	100
6	F	131/151 (87%)	131 (100%)	0	100	100
7	G	120/123 (98%)	120 (100%)	0	100	100
8	H	101/101 (100%)	101 (100%)	0	100	100
9	I	71/110 (64%)	71 (100%)	0	100	100
10	J	99/100 (99%)	99 (100%)	0	100	100
11	K	98/100 (98%)	98 (100%)	0	100	100
12	L	95/97 (98%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	M	83/84 (99%)	83 (100%)	0	100 100
14	N	90/93 (97%)	90 (100%)	0	100 100
15	O	82/85 (96%)	82 (100%)	0	100 100
16	P	82/87 (94%)	82 (100%)	0	100 100
17	Q	38/74 (51%)	38 (100%)	0	100 100
18	R	56/57 (98%)	56 (100%)	0	100 100
19	S	52/53 (98%)	52 (100%)	0	100 100
20	T	38/53 (72%)	37 (97%)	1 (3%)	41 68
21	U	39/39 (100%)	39 (100%)	0	100 100
22	V	227/244 (93%)	227 (100%)	0	100 100
23	W	343/371 (92%)	341 (99%)	2 (1%)	84 91
24	Y	138/185 (75%)	124 (90%)	14 (10%)	6 23
All	All	2517/2772 (91%)	2500 (99%)	17 (1%)	80 90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	16	ARG
23	W	390	VAL
23	W	391	LYS
24	Y	56	ASP
24	Y	57	GLN
24	Y	59	ILE
24	Y	60	ARG
24	Y	65	LEU
24	Y	67	ASN
24	Y	121	MET
24	Y	123	GLU
24	Y	127	ILE
24	Y	130	VAL
24	Y	198	LYS
24	Y	200	LYS
24	Y	205	LYS
24	Y	207	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	143	ASN
3	C	264	ASN
5	E	67	GLN
9	I	17	ASN
9	I	68	ASN
10	J	76	ASN
12	L	72	ASN
13	M	18	GLN
16	P	2	HIS
20	T	19	HIS
22	V	130	ASN
23	W	185	ASN
23	W	312	ASN
23	W	318	GLN
23	W	349	ASN
23	W	357	ASN
24	Y	55	ASN
24	Y	57	GLN
24	Y	67	ASN
24	Y	106	GLN
24	Y	188	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2555/2927 (87%)	825 (32%)	64 (2%)
2	B	111/119 (93%)	66 (59%)	6 (5%)
All	All	2666/3046 (87%)	891 (33%)	70 (2%)

All (891) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	28	A
1	A	34	U
1	A	36	G
1	A	39	C
1	A	43	G
1	A	51	G
1	A	55	G
1	A	59	G
1	A	60	G

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Mol	Chain	Res	Type
1	A	63	G
1	A	67	A
1	A	71	A
1	A	75	G
1	A	87	U
1	A	90	A
1	A	91	A
1	A	92	G
1	A	94	A
1	A	98	U
1	A	99	U
1	A	100	U
1	A	101	G
1	A	117	A
1	A	119	U
1	A	133	A
1	A	157	U
1	A	158	C
1	A	159	U
1	A	161	A
1	A	162	A
1	A	163	U
1	A	164	U
1	A	166	A
1	A	176	A
1	A	177	G
1	A	184	G
1	A	185	A
1	A	199	A
1	A	200	A
1	A	201	C
1	A	202	A
1	A	203	U
1	A	204	C
1	A	206	A
1	A	207	A
1	A	216	A
1	A	219	A
1	A	225	A
1	A	226	A
1	A	228	C
1	A	229	A

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Mol	Chain	Res	Type
1	A	230	A
1	A	231	A
1	A	232	U
1	A	233	G
1	A	248	G
1	A	251	G
1	A	252	C
1	A	253	G
1	A	262	G
1	A	266	U
1	A	268	A
1	A	269	G
1	A	270	C
1	A	272	C
1	A	273	A
1	A	274	A
1	A	275	A
1	A	276	C
1	A	277	C
1	A	278	A
1	A	280	G
1	A	281	A
1	A	282	G
1	A	287	G
1	A	288	C
1	A	289	C
1	A	290	U
1	A	291	C
1	A	293	U
1	A	294	G
1	A	297	G
1	A	298	U
1	A	299	U
1	A	300	G
1	A	301	U
1	A	302	A
1	A	303	G
1	A	304	G
1	A	306	C
1	A	307	A
1	A	309	U
1	A	314	A

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Mol	Chain	Res	Type
1	A	315	C
1	A	316	G
1	A	317	G
1	A	318	A
1	A	321	U
1	A	322	A
1	A	324	A
1	A	327	G
1	A	328	G
1	A	329	A
1	A	330	A
1	A	337	A
1	A	338	G
1	A	344	G
1	A	345	A
1	A	346	G
1	A	348	U
1	A	355	A
1	A	360	C
1	A	361	G
1	A	368	G
1	A	374	A
1	A	378	C
1	A	382	G
1	A	386	U
1	A	388	A
1	A	392	C
1	A	393	U
1	A	396	G
1	A	399	C
1	A	402	U
1	A	405	U
1	A	408	G
1	A	410	G
1	A	412	A
1	A	413	U
1	A	414	C
1	A	415	C
1	A	416	U
1	A	418	A
1	A	419	G
1	A	420	U

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Mol	Chain	Res	Type
1	A	424	G
1	A	426	G
1	A	431	A
1	A	433	G
1	A	434	U
1	A	435	G
1	A	437	A
1	A	438	A
1	A	439	U
1	A	440	U
1	A	445	C
1	A	446	G
1	A	449	A
1	A	450	U
1	A	453	G
1	A	459	A
1	A	462	A
1	A	463	U
1	A	464	C
1	A	474	U
1	A	482	C
1	A	487	G
1	A	502	C
1	A	503	C
1	A	504	A
1	A	526	A
1	A	528	G
1	A	538	A
1	A	550	G
1	A	551	A
1	A	554	U
1	A	555	C
1	A	556	C
1	A	568	G
1	A	576	G
1	A	577	U
1	A	578	A
1	A	579	G
1	A	584	A
1	A	588	C
1	A	592	A
1	A	595	G

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Mol	Chain	Res	Type
1	A	607	G
1	A	619	A
1	A	632	U
1	A	647	A
1	A	651	U
1	A	658	A
1	A	673	A
1	A	678	A
1	A	680	G
1	A	681	C
1	A	683	A
1	A	684	G
1	A	685	U
1	A	686	C
1	A	688	G
1	A	690	A
1	A	691	U
1	A	692	A
1	A	694	G
1	A	696	C
1	A	697	G
1	A	698	C
1	A	699	A
1	A	700	U
1	A	701	G
1	A	715	A
1	A	722	A
1	A	732	A
1	A	733	U
1	A	734	C
1	A	735	U
1	A	760	G
1	A	761	U
1	A	762	A
1	A	765	A
1	A	766	C
1	A	767	U
1	A	768	G
1	A	777	C
1	A	793	U
1	A	794	U
1	A	795	G

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Mol	Chain	Res	Type
1	A	799	A
1	A	811	A
1	A	812	G
1	A	822	G
1	A	823	G
1	A	824	G
1	A	829	A
1	A	830	A
1	A	831	U
1	A	837	U
1	A	838	C
1	A	839	G
1	A	841	A
1	A	848	G
1	A	852	G
1	A	858	U
1	A	859	C
1	A	866	A
1	A	870	A
1	A	871	G
1	A	873	U
1	A	874	U
1	A	875	U
1	A	876	A
1	A	881	U
1	A	882	A
1	A	892	U
1	A	901	U
1	A	902	G
1	A	903	G
1	A	904	A
1	A	905	G
1	A	906	G
1	A	907	U
1	A	908	A
1	A	910	A
1	A	912	C
1	A	913	A
1	A	914	C
1	A	915	U
1	A	961	C
1	A	964	A

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Mol	Chain	Res	Type
1	A	966	U
1	A	967	G
1	A	968	C
1	A	969	C
1	A	970	A
1	A	972	U
1	A	973	G
1	A	975	C
1	A	976	U
1	A	978	A
1	A	987	A
1	A	992	G
1	A	999	A
1	A	1000	G
1	A	1002	G
1	A	1003	A
1	A	1004	U
1	A	1005	A
1	A	1009	U
1	A	1010	C
1	A	1019	A
1	A	1020	A
1	A	1027	A
1	A	1029	A
1	A	1041	C
1	A	1042	A
1	A	1049	G
1	A	1051	C
1	A	1054	A
1	A	1055	A
1	A	1057	G
1	A	1058	U
1	A	1059	A
1	A	1063	G
1	A	1068	G
1	A	1069	U
1	A	1071	G
1	A	1072	A
1	A	1073	A
1	A	1077	G
1	A	1078	A
1	A	1079	U

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Mol	Chain	Res	Type
1	A	1081	U
1	A	1082	G
1	A	1084	A
1	A	1085	G
1	A	1086	U
1	A	1089	C
1	A	1090	U
1	A	1091	U
1	A	1093	G
1	A	1094	A
1	A	1095	C
1	A	1096	A
1	A	1097	A
1	A	1098	C
1	A	1099	C
1	A	1100	A
1	A	1101	G
1	A	1151	U
1	A	1152	G
1	A	1153	G
1	A	1156	G
1	A	1157	A
1	A	1158	G
1	A	1161	A
1	A	1165	U
1	A	1167	C
1	A	1172	A
1	A	1173	A
1	A	1174	A
1	A	1175	A
1	A	1176	U
1	A	1179	A
1	A	1180	C
1	A	1181	C
1	A	1185	G
1	A	1187	U
1	A	1188	A
1	A	1192	G
1	A	1209	G
1	A	1215	U
1	A	1216	C
1	A	1217	U

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Mol	Chain	Res	Type
1	A	1218	U
1	A	1219	C
1	A	1220	G
1	A	1245	G
1	A	1246	G
1	A	1247	G
1	A	1248	C
1	A	1251	U
1	A	1252	G
1	A	1260	A
1	A	1276	G
1	A	1278	G
1	A	1287	A
1	A	1289	U
1	A	1293	A
1	A	1294	A
1	A	1296	G
1	A	1312	A
1	A	1314	A
1	A	1315	G
1	A	1328	C
1	A	1339	A
1	A	1340	A
1	A	1344	C
1	A	1345	U
1	A	1346	A
1	A	1352	U
1	A	1360	A
1	A	1363	G
1	A	1364	C
1	A	1376	G
1	A	1380	U
1	A	1388	A
1	A	1391	U
1	A	1404	A
1	A	1405	A
1	A	1407	G
1	A	1414	G
1	A	1418	U
1	A	1423	A
1	A	1424	A
1	A	1425	C

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Mol	Chain	Res	Type
1	A	1428	G
1	A	1434	A
1	A	1435	U
1	A	1436	U
1	A	1439	U
1	A	1448	U
1	A	1449	C
1	A	1451	U
1	A	1452	C
1	A	1455	C
1	A	1456	A
1	A	1458	U
1	A	1459	U
1	A	1460	G
1	A	1462	G
1	A	1465	A
1	A	1467	G
1	A	1473	A
1	A	1474	C
1	A	1479	G
1	A	1480	A
1	A	1481	G
1	A	1483	A
1	A	1484	U
1	A	1491	A
1	A	1495	C
1	A	1496	G
1	A	1497	G
1	A	1498	U
1	A	1499	A
1	A	1501	U
1	A	1503	G
1	A	1504	A
1	A	1505	U
1	A	1506	A
1	A	1507	U
1	A	1513	U
1	A	1516	A
1	A	1520	A
1	A	1521	G
1	A	1524	A
1	A	1525	G

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Mol	Chain	Res	Type
1	A	1526	G
1	A	1527	C
1	A	1528	U
1	A	1529	G
1	A	1533	A
1	A	1534	A
1	A	1539	C
1	A	1540	A
1	A	1543	U
1	A	1547	U
1	A	1553	A
1	A	1554	U
1	A	1555	A
1	A	1556	A
1	A	1559	C
1	A	1561	G
1	A	1567	U
1	A	1571	G
1	A	1572	G
1	A	1573	C
1	A	1576	G
1	A	1577	C
1	A	1578	G
1	A	1580	A
1	A	1589	G
1	A	1596	U
1	A	1598	C
1	A	1600	G
1	A	1607	C
1	A	1614	A
1	A	1617	A
1	A	1626	U
1	A	1630	G
1	A	1631	A
1	A	1632	G
1	A	1634	U
1	A	1638	A
1	A	1652	C
1	A	1653	A
1	A	1655	A
1	A	1657	C
1	A	1667	A

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Mol	Chain	Res	Type
1	A	1677	A
1	A	1678	G
1	A	1679	A
1	A	1685	A
1	A	1692	U
1	A	1693	C
1	A	1697	A
1	A	1719	G
1	A	1728	C
1	A	1729	C
1	A	1733	U
1	A	1745	A
1	A	1758	U
1	A	1759	U
1	A	1760	A
1	A	1761	G
1	A	1774	A
1	A	1777	G
1	A	1778	A
1	A	1779	G
1	A	1787	G
1	A	1791	A
1	A	1792	G
1	A	1793	G
1	A	1802	A
1	A	1810	G
1	A	1811	C
1	A	1813	A
1	A	1829	C
1	A	1831	A
1	A	1834	C
1	A	1838	A
1	A	1847	U
1	A	1850	A
1	A	1858	A
1	A	1860	G
1	A	1861	C
1	A	1862	C
1	A	1863	U
1	A	2005	C
1	A	2014	G
1	A	2020	U

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Mol	Chain	Res	Type
1	A	2021	G
1	A	2022	U
1	A	2023	C
1	A	2024	U
1	A	2026	A
1	A	2050	G
1	A	2052	A
1	A	2055	U
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	U
1	A	2072	C
1	A	2085	G
1	A	2089	A
1	A	2090	G
1	A	2091	A
1	A	2092	C
1	A	2093	C
1	A	2096	G
1	A	2097	U
1	A	2098	G
1	A	2104	U
1	A	2105	U
1	A	2106	A
1	A	2108	U
1	A	2109	G
1	A	2110	C
1	A	2111	A
1	A	2114	C
1	A	2115	U
1	A	2117	A
1	A	2129	G
1	A	2134	A
1	A	2138	U
1	A	2140	U
1	A	2142	C
1	A	2144	G
1	A	2146	A
1	A	2147	U
1	A	2149	G

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Mol	Chain	Res	Type
1	A	2150	G
1	A	2151	U
1	A	2152	A
1	A	2153	G
1	A	2155	A
1	A	2156	G
1	A	2157	C
1	A	2189	G
1	A	2190	C
1	A	2193	C
1	A	2195	G
1	A	2196	U
1	A	2197	G
1	A	2198	G
1	A	2199	G
1	A	2200	A
1	A	2201	U
1	A	2202	A
1	A	2203	C
1	A	2205	A
1	A	2206	C
1	A	2209	U
1	A	2211	G
1	A	2214	G
1	A	2216	A
1	A	2218	U
1	A	2222	C
1	A	2224	U
1	A	2228	A
1	A	2232	G
1	A	2233	C
1	A	2239	U
1	A	2240	U
1	A	2241	A
1	A	2243	C
1	A	2252	A
1	A	2253	G
1	A	2254	A
1	A	2255	C
1	A	2260	U
1	A	2262	A
1	A	2263	G

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Mol	Chain	Res	Type
1	A	2264	G
1	A	2266	G
1	A	2267	G
1	A	2268	G
1	A	2272	U
1	A	2273	U
1	A	2274	U
1	A	2292	C
1	A	2293	C
1	A	2295	A
1	A	2296	A
1	A	2297	A
1	A	2298	A
1	A	2308	G
1	A	2311	G
1	A	2312	C
1	A	2313	C
1	A	2314	C
1	A	2315	A
1	A	2318	G
1	A	2320	U
1	A	2322	C
1	A	2323	C
1	A	2324	C
1	A	2325	U
1	A	2326	C
1	A	2327	A
1	A	2348	C
1	A	2349	A
1	A	2350	G
1	A	2351	A
1	A	2352	G
1	A	2353	U
1	A	2354	G
1	A	2356	A
1	A	2358	A
1	A	2359	G
1	A	2362	A
1	A	2363	C
1	A	2364	A
1	A	2365	A
1	A	2366	G

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Mol	Chain	Res	Type
1	A	2367	G
1	A	2368	G
1	A	2369	A
1	A	2372	U
1	A	2373	U
1	A	2374	G
1	A	2375	A
1	A	2376	C
1	A	2377	U
1	A	2378	G
1	A	2395	A
1	A	2398	A
1	A	2399	G
1	A	2400	G
1	A	2401	G
1	A	2402	A
1	A	2403	C
1	A	2404	G
1	A	2406	A
1	A	2410	C
1	A	2411	G
1	A	2412	G
1	A	2413	G
1	A	2414	C
1	A	2415	U
1	A	2416	U
1	A	2417	A
1	A	2418	G
1	A	2422	U
1	A	2424	C
1	A	2425	G
1	A	2427	U
1	A	2428	G
1	A	2431	U
1	A	2432	C
1	A	2433	C
1	A	2434	G
1	A	2435	C
1	A	2437	U
1	A	2441	A
1	A	2442	G
1	A	2443	G

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Mol	Chain	Res	Type
1	A	2445	C
1	A	2446	C
1	A	2447	A
1	A	2449	C
1	A	2450	G
1	A	2451	C
1	A	2452	U
1	A	2453	C
1	A	2454	A
1	A	2456	C
1	A	2457	G
1	A	2458	G
1	A	2459	A
1	A	2460	U
1	A	2462	A
1	A	2463	A
1	A	2464	A
1	A	2466	C
1	A	2467	U
1	A	2468	A
1	A	2469	C
1	A	2470	C
1	A	2474	G
1	A	2475	G
1	A	2489	U
1	A	2490	C
1	A	2492	C
1	A	2493	C
1	A	2494	C
1	A	2495	C
1	A	2516	G
1	A	2517	A
1	A	2518	G
1	A	2519	G
1	A	2522	U
1	A	2523	G
1	A	2525	C
1	A	2526	A
1	A	2527	C
1	A	2541	C
1	A	2542	A
1	A	2547	A

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Mol	Chain	Res	Type
1	A	2548	U
1	A	2549	C
1	A	2555	G
1	A	2556	C
1	A	2557	U
1	A	2560	A
1	A	2563	C
1	A	2577	G
1	A	2581	U
1	A	2582	G
1	A	2583	U
1	A	2584	U
1	A	2585	C
1	A	2586	G
1	A	2588	C
1	A	2595	A
1	A	2596	G
1	A	2601	A
1	A	2602	C
1	A	2611	G
1	A	2612	G
1	A	2613	U
1	A	2615	C
1	A	2616	A
1	A	2619	A
1	A	2620	C
1	A	2621	G
1	A	2625	U
1	A	2628	G
1	A	2629	A
1	A	2631	A
1	A	2632	G
1	A	2634	U
1	A	2639	C
1	A	2642	U
1	A	2648	U
1	A	2658	A
1	A	2660	G
1	A	2661	A
1	A	2668	A
1	A	2675	C
1	A	2681	U

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Mol	Chain	Res	Type
1	A	2684	G
1	A	2686	A
1	A	2689	A
1	A	2690	G
1	A	2693	G
1	A	2694	A
1	A	2696	C
1	A	2697	G
1	A	2698	G
1	A	2714	G
1	A	2718	U
1	A	2720	C
1	A	2731	G
1	A	2734	A
1	A	2736	G
1	A	2743	G
1	A	2755	U
1	A	2762	A
1	A	2766	G
1	A	2767	A
1	A	2773	G
1	A	2775	U
1	A	2776	G
1	A	2777	A
1	A	2780	G
1	A	2781	C
1	A	2782	A
1	A	2783	U
1	A	2784	C
1	A	2786	A
1	A	2787	A
1	A	2788	G
1	A	2794	A
1	A	2795	G
1	A	2796	C
1	A	2797	C
1	A	2807	A
1	A	2811	G
1	A	2813	U
1	A	2818	C
1	A	2819	A
1	A	2820	U

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Mol	Chain	Res	Type
1	A	2823	C
1	A	2825	C
1	A	2826	A
1	A	2837	A
1	A	2845	A
1	A	2858	U
1	A	2859	G
1	A	2860	A
1	A	2868	G
1	A	2874	G
1	A	2892	G
1	A	2897	G
1	A	2908	A
1	A	2910	C
1	A	2916	A
1	A	2924	A
1	A	2925	C
2	B	5	G
2	B	6	U
2	B	8	G
2	B	9	C
2	B	10	G
2	B	11	A
2	B	12	U
2	B	13	A
2	B	14	G
2	B	19	G
2	B	20	A
2	B	21	G
2	B	22	G
2	B	23	U
2	B	26	C
2	B	27	A
2	B	28	C
2	B	32	U
2	B	34	C
2	B	38	U
2	B	39	A
2	B	40	C
2	B	41	C
2	B	42	G
2	B	43	A

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Mol	Chain	Res	Type
2	B	44	A
2	B	46	A
2	B	48	G
2	B	49	G
2	B	51	A
2	B	54	U
2	B	55	A
2	B	59	U
2	B	60	C
2	B	61	U
2	B	62	U
2	B	63	C
2	B	64	A
2	B	67	G
2	B	68	C
2	B	69	C
2	B	71	A
2	B	74	G
2	B	75	U
2	B	76	A
2	B	78	U
2	B	79	C
2	B	82	G
2	B	83	G
2	B	84	G
2	B	85	U
2	B	86	U
2	B	87	U
2	B	88	C
2	B	89	C
2	B	91	C
2	B	95	U
2	B	96	G
2	B	97	A
2	B	101	U
2	B	104	G
2	B	106	C
2	B	107	G
2	B	108	C
2	B	111	C
2	B	112	C

All (70) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	58	G
1	A	90	A
1	A	97	C
1	A	160	G
1	A	184	G
1	A	230	A
1	A	267	C
1	A	268	A
1	A	271	C
1	A	288	C
1	A	296	G
1	A	303	G
1	A	317	G
1	A	377	G
1	A	414	C
1	A	433	G
1	A	439	U
1	A	462	A
1	A	503	C
1	A	525	A
1	A	549	A
1	A	578	A
1	A	677	A
1	A	682	G
1	A	837	U
1	A	968	C
1	A	1155	C
1	A	1173	A
1	A	1245	G
1	A	1250	G
1	A	1339	A
1	A	1351	U
1	A	1362	G
1	A	1434	A
1	A	1438	C
1	A	1455	C
1	A	1478	G
1	A	1526	G
1	A	1595	U
1	A	1652	C
1	A	1837	U
1	A	1846	G
1	A	2090	G

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Mol	Chain	Res	Type
1	A	2091	A
1	A	2109	G
1	A	2150	G
1	A	2254	A
1	A	2272	U
1	A	2292	C
1	A	2321	U
1	A	2323	C
1	A	2326	C
1	A	2351	A
1	A	2398	A
1	A	2405	A
1	A	2409	U
1	A	2468	A
1	A	2583	U
1	A	2585	C
1	A	2683	A
1	A	2779	A
1	A	2785	U
1	A	2812	A
1	A	2858	U
2	B	7	G
2	B	37	A
2	B	38	U
2	B	47	C
2	B	53	U
2	B	63	C

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)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	GNP	V	301	-	29,34,34	1.56	7 (24%)	33,54,54	2.20	5 (15%)
25	GNP	W	502	-	29,34,34	1.65	7 (24%)	33,54,54	2.22	6 (18%)
25	GNP	W	501	-	29,34,34	1.62	7 (24%)	33,54,54	2.20	5 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GNP	V	301	-	-	6/14/38/38	0/3/3/3
25	GNP	W	502	-	-	5/14/38/38	0/3/3/3
25	GNP	W	501	-	-	6/14/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	W	502	GNP	PB-O3A	4.72	1.64	1.59
25	W	501	GNP	PB-O3A	4.49	1.64	1.59
25	V	301	GNP	PB-O3A	4.05	1.64	1.59
25	W	502	GNP	PB-O1B	3.22	1.51	1.46
25	W	501	GNP	PB-O1B	3.11	1.50	1.46
25	W	502	GNP	C6-N1	3.09	1.38	1.33
25	W	501	GNP	C6-N1	3.07	1.38	1.33
25	V	301	GNP	C6-N1	3.06	1.38	1.33
25	V	301	GNP	PB-O1B	2.97	1.50	1.46
25	W	502	GNP	PG-N3B	2.94	1.71	1.63
25	W	501	GNP	PG-N3B	2.87	1.70	1.63
25	W	501	GNP	PG-O1G	2.79	1.50	1.46
25	V	301	GNP	PG-N3B	2.73	1.70	1.63
25	V	301	GNP	PG-O1G	2.71	1.50	1.46
25	W	502	GNP	PG-O1G	2.67	1.50	1.46
25	V	301	GNP	PB-O2B	-2.27	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	W	502	GNP	PB-O2B	-2.27	1.50	1.56
25	W	501	GNP	PB-O2B	-2.23	1.50	1.56
25	W	502	GNP	C5-C6	2.11	1.45	1.41
25	W	501	GNP	C5-C6	2.01	1.44	1.41
25	V	301	GNP	C5-C6	2.00	1.44	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	W	501	GNP	C5-C6-N1	-8.60	111.92	123.42
25	W	502	GNP	C5-C6-N1	-8.60	111.93	123.42
25	V	301	GNP	C5-C6-N1	-8.55	111.98	123.42
25	W	501	GNP	C2-N1-C6	6.64	125.20	115.96
25	W	502	GNP	C2-N1-C6	6.64	125.19	115.96
25	V	301	GNP	C2-N1-C6	6.59	125.12	115.96
25	V	301	GNP	N3-C2-N1	-2.91	123.51	127.21
25	W	501	GNP	N3-C2-N1	-2.89	123.53	127.21
25	W	502	GNP	N3-C2-N1	-2.88	123.54	127.21
25	W	501	GNP	C2-N3-C4	-2.44	112.86	115.48
25	W	502	GNP	C2-N3-C4	-2.43	112.87	115.48
25	V	301	GNP	C2-N3-C4	-2.41	112.88	115.48
25	V	301	GNP	O1G-PG-N3B	-2.37	108.27	111.77
25	W	501	GNP	O1B-PB-N3B	-2.14	108.62	111.77
25	W	502	GNP	O1B-PB-N3B	-2.12	108.65	111.77
25	W	502	GNP	O2A-PA-O3A	2.04	112.78	107.27

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	V	301	GNP	PB-N3B-PG-O1G
25	V	301	GNP	PG-N3B-PB-O1B
25	V	301	GNP	PA-O3A-PB-O2B
25	V	301	GNP	C5'-O5'-PA-O3A
25	W	501	GNP	PG-N3B-PB-O1B
25	W	502	GNP	PB-N3B-PG-O1G
25	W	502	GNP	PG-N3B-PB-O1B
25	W	502	GNP	PG-N3B-PB-O3A
25	W	502	GNP	PA-O3A-PB-O2B
25	W	501	GNP	O4'-C4'-C5'-O5'
25	W	501	GNP	C3'-C4'-C5'-O5'
25	V	301	GNP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
25	W	501	GNP	C5'-O5'-PA-O3A
25	W	501	GNP	C5'-O5'-PA-O1A
25	W	501	GNP	C5'-O5'-PA-O2A
25	V	301	GNP	PA-O3A-PB-O1B
25	W	502	GNP	PA-O3A-PB-O1B

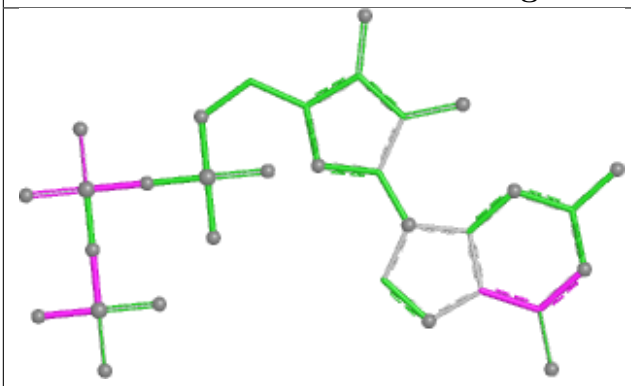
There are no ring outliers.

2 monomers are involved in 5 short contacts:

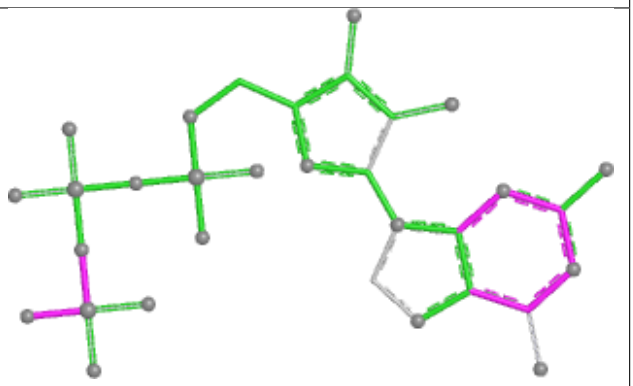
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	W	502	GNP	2	0
25	W	501	GNP	3	0

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

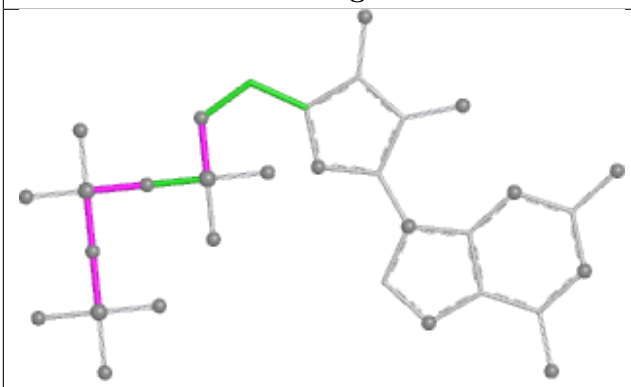
Ligand GNP V 301



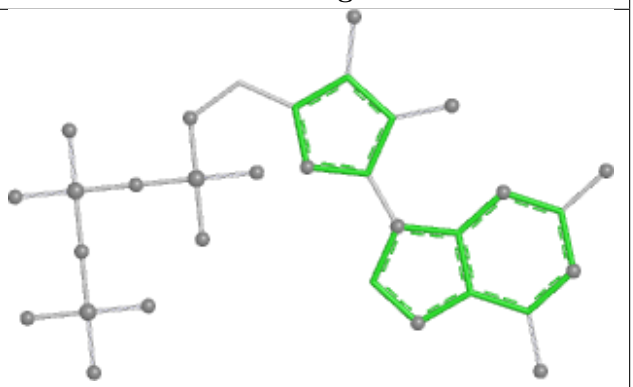
Bond lengths



Bond angles

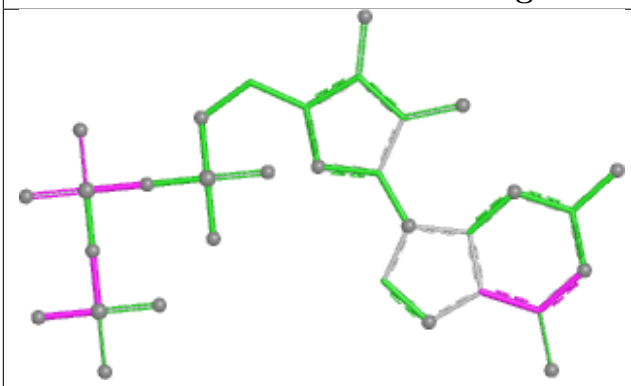


Torsions

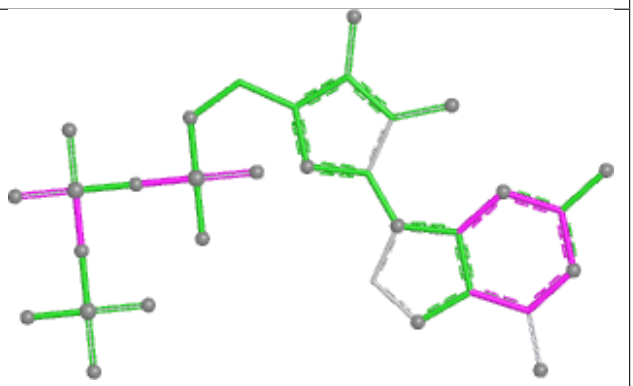


Rings

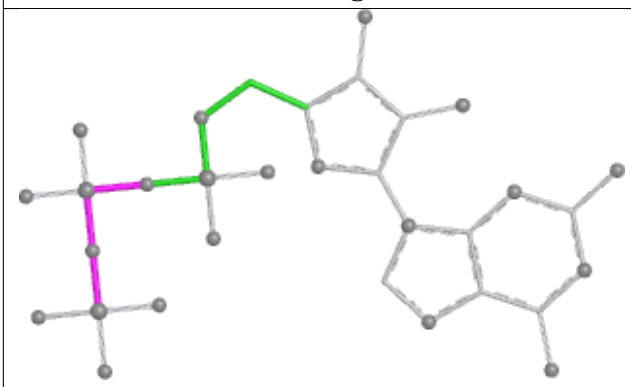
Ligand GNP W 502



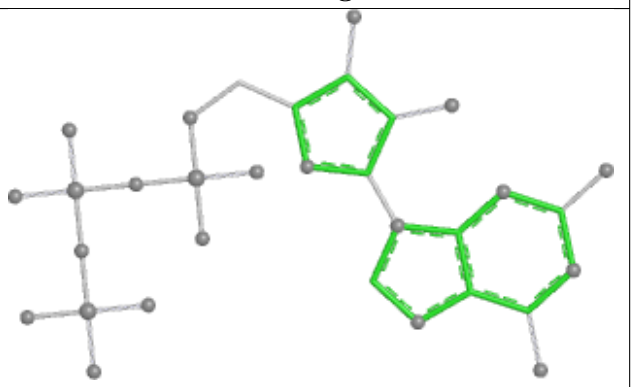
Bond lengths



Bond angles

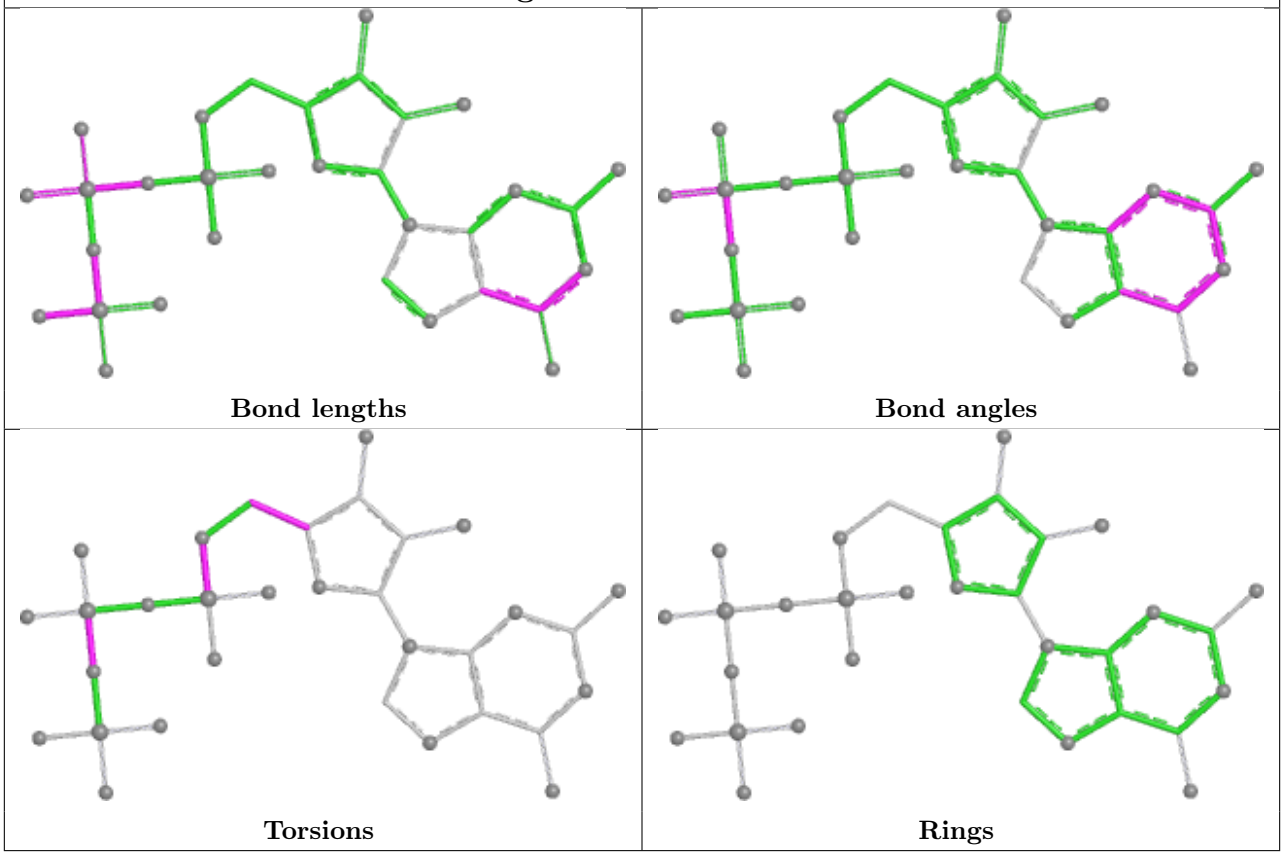


Torsions



Rings

Ligand GNP W 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

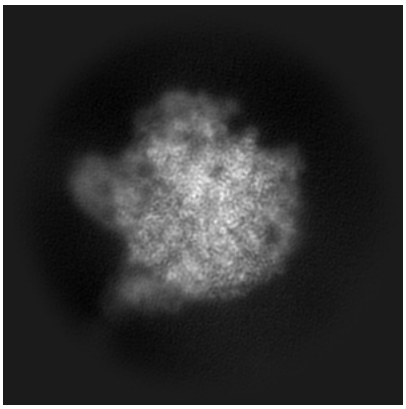
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44871. These allow visual inspection of the internal detail of the map and identification of artifacts.

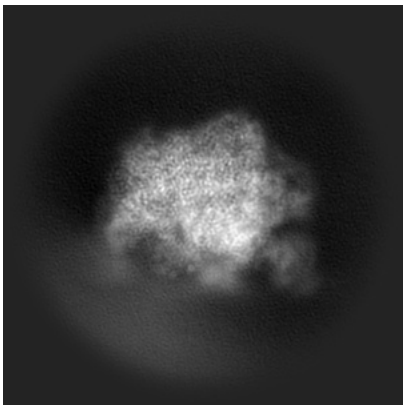
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

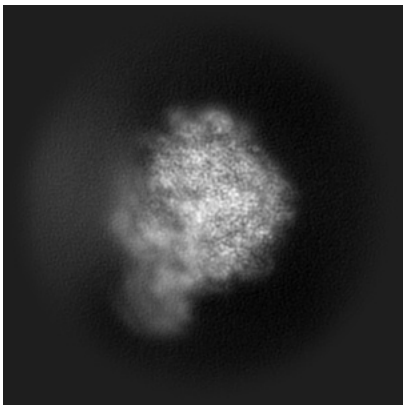
6.1.1 Primary map



X

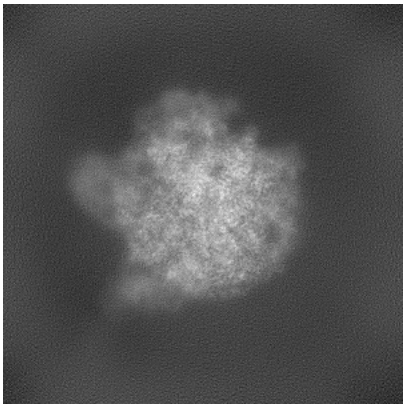


Y

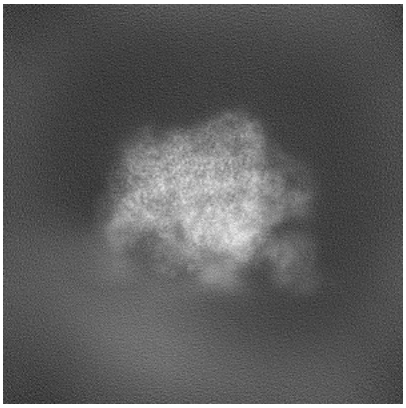


Z

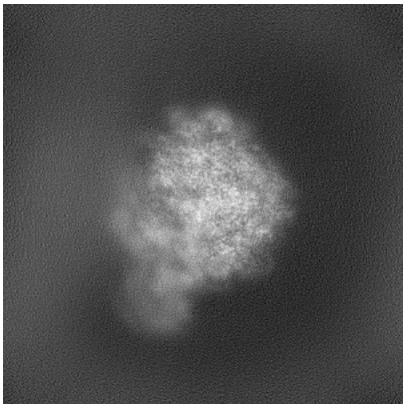
6.1.2 Raw map



X



Y

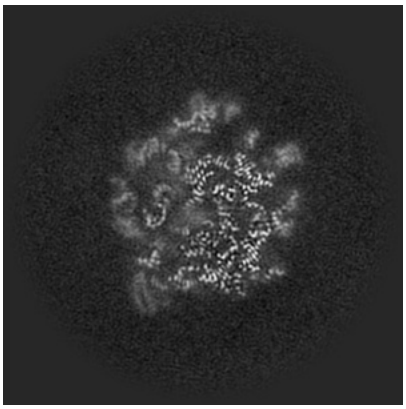


Z

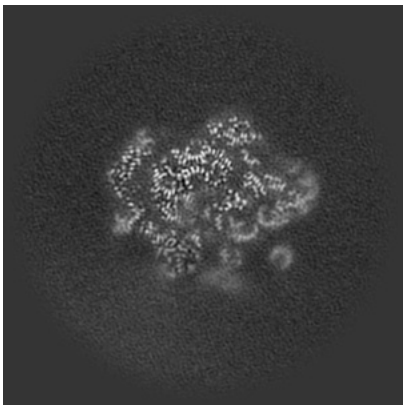
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

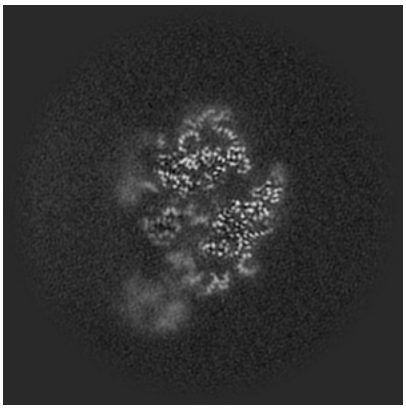
6.2.1 Primary map



X Index: 224

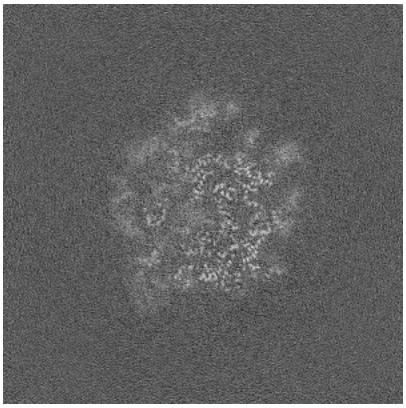


Y Index: 224

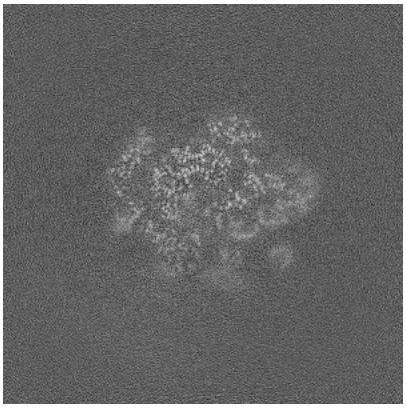


Z Index: 224

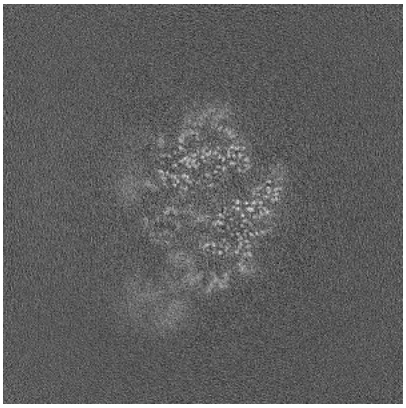
6.2.2 Raw map



X Index: 224



Y Index: 224

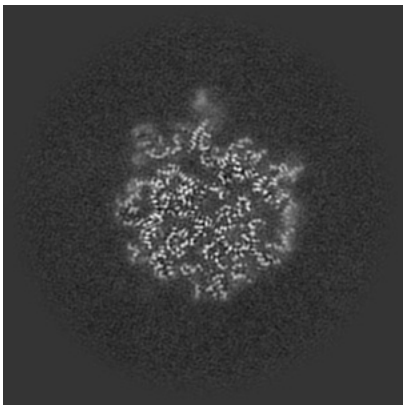


Z Index: 224

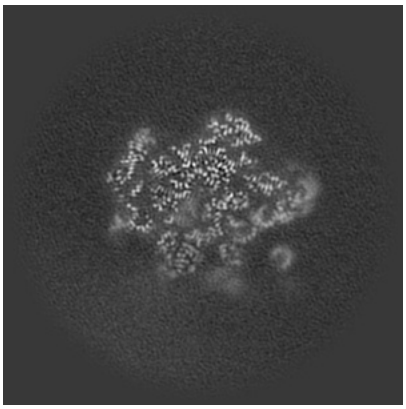
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

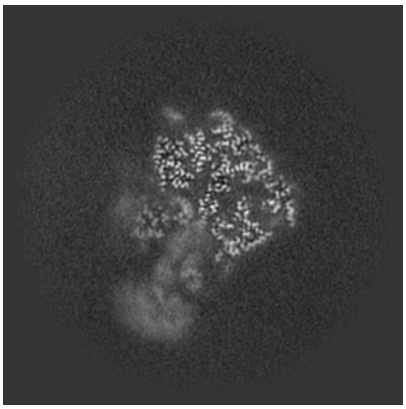
6.3.1 Primary map



X Index: 246

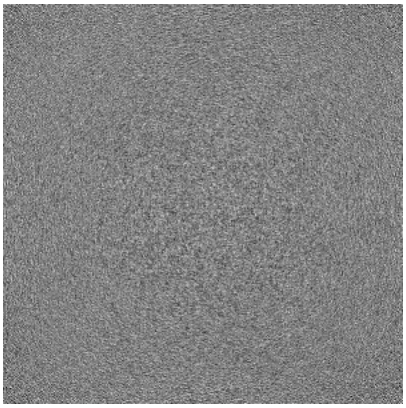


Y Index: 221

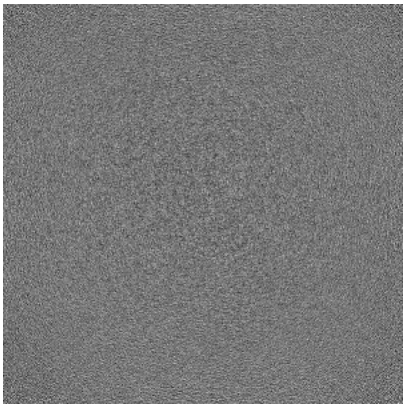


Z Index: 255

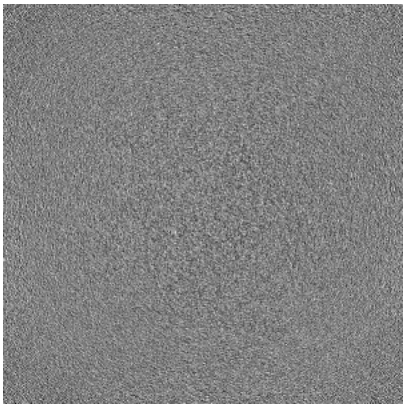
6.3.2 Raw map



X Index: 0



Y Index: 0

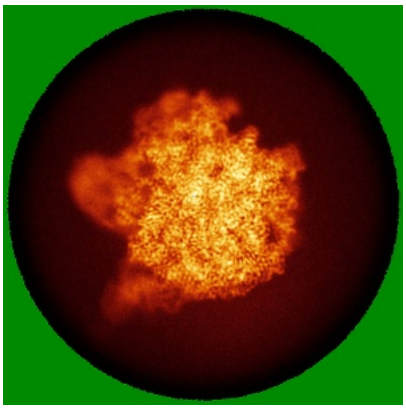


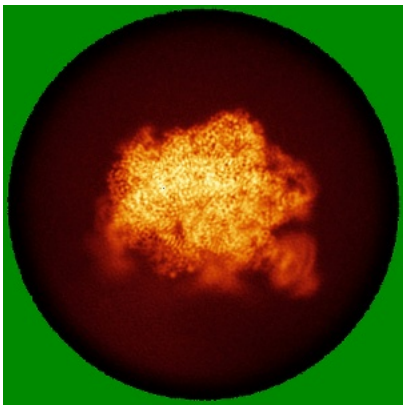
Z Index: 0

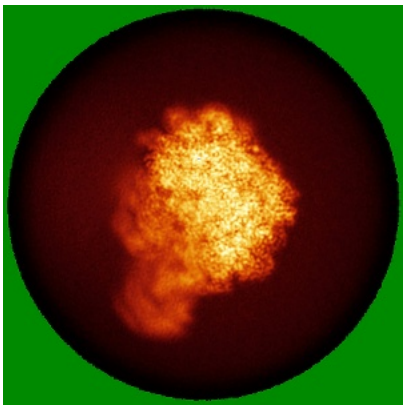
The images above show the largest variance slices of the map in three orthogonal directions.

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

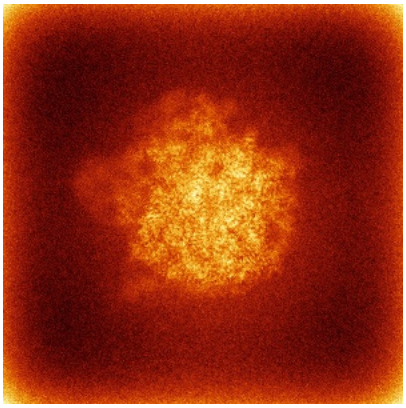
6.4.1 Primary map

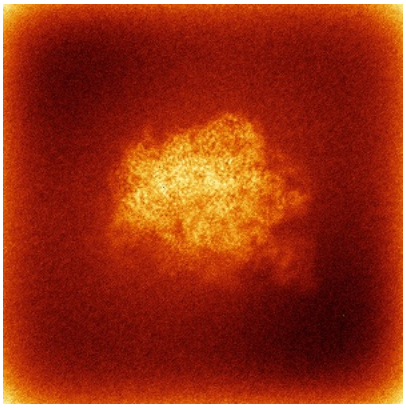

X

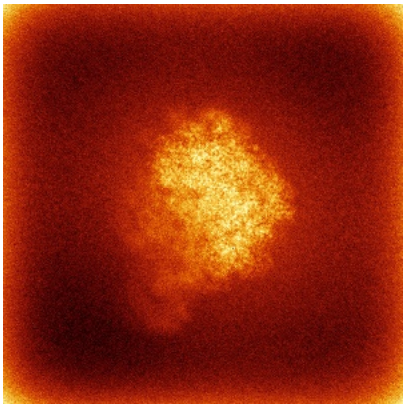

Y


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.

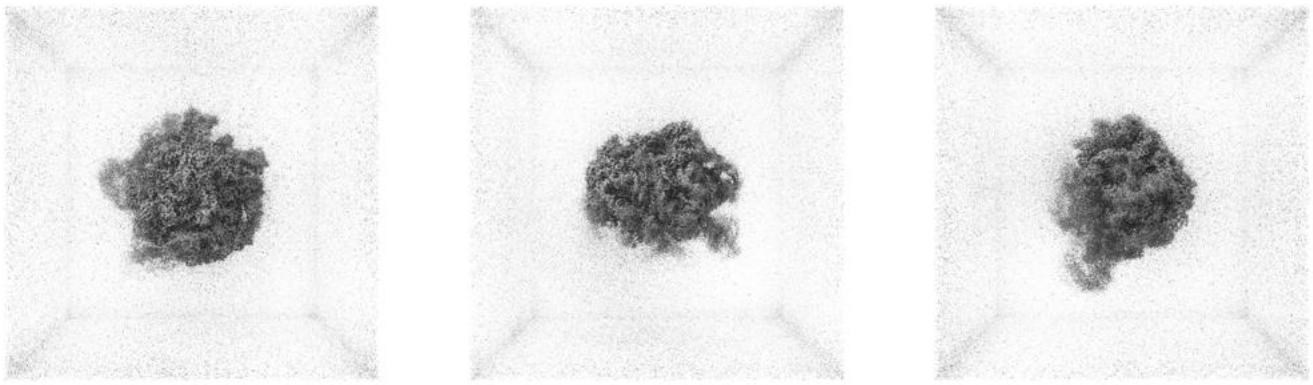
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.146. 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



X Y Z

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.

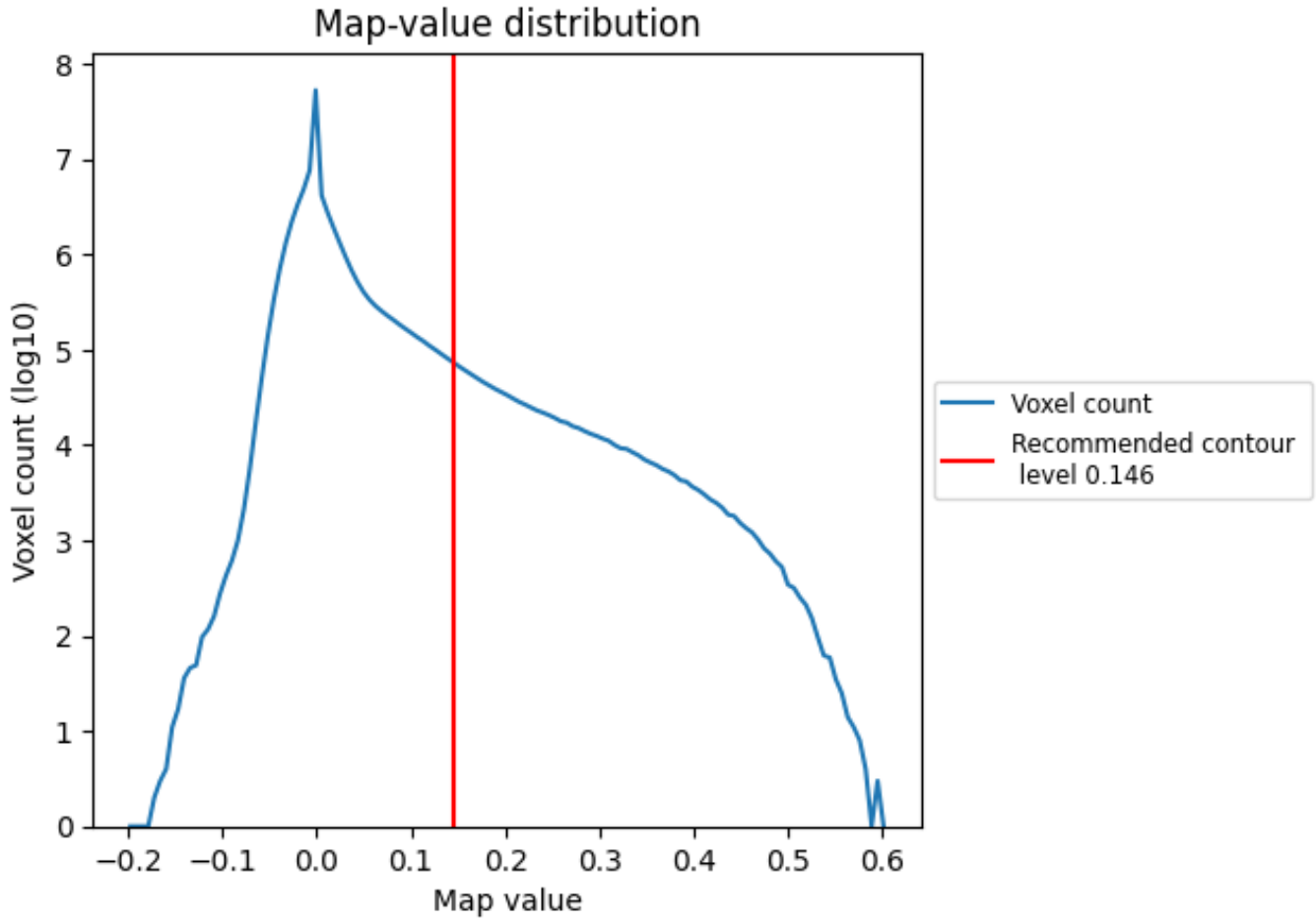
6.6 Mask visualisation (i)

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

7 Map analysis

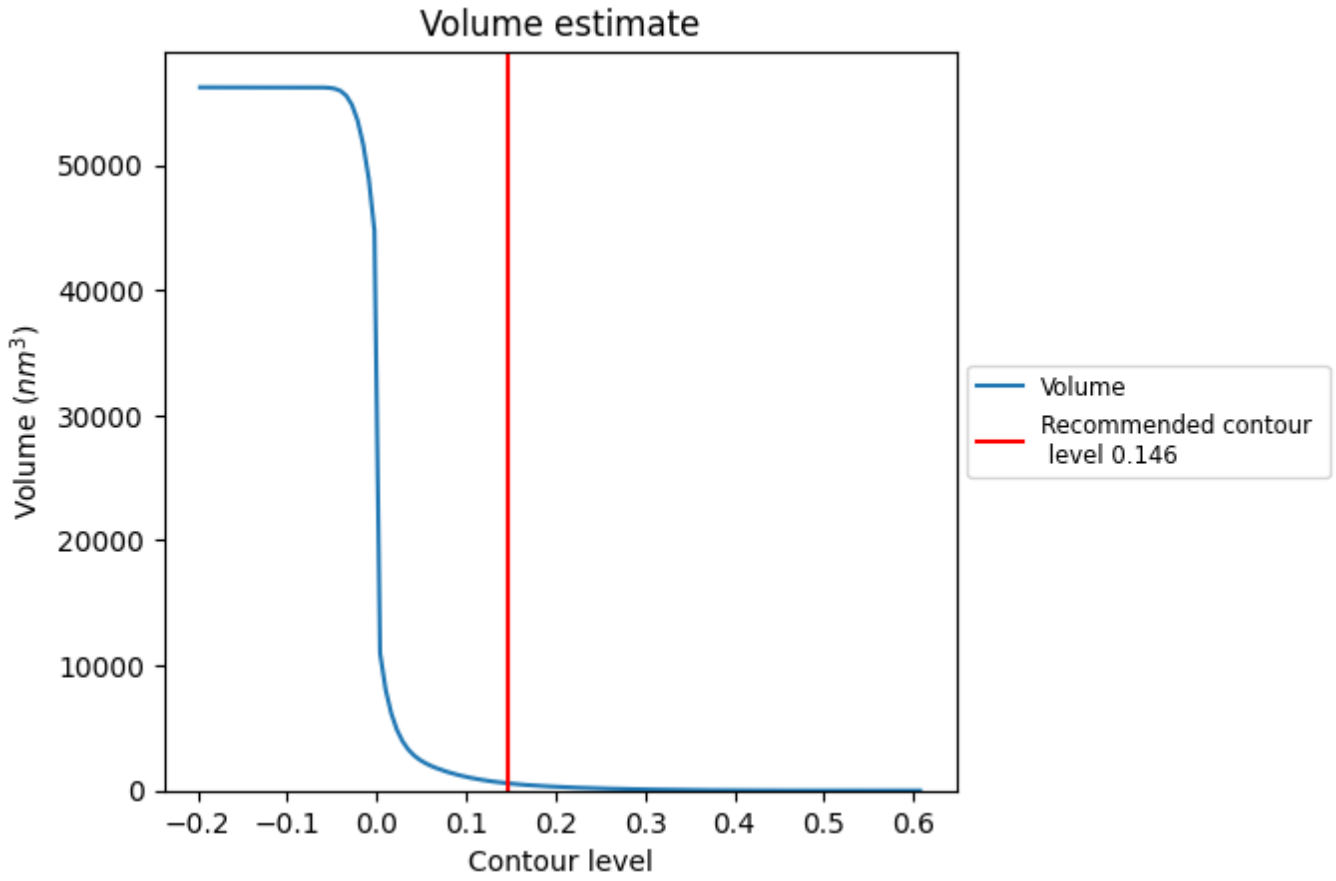
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

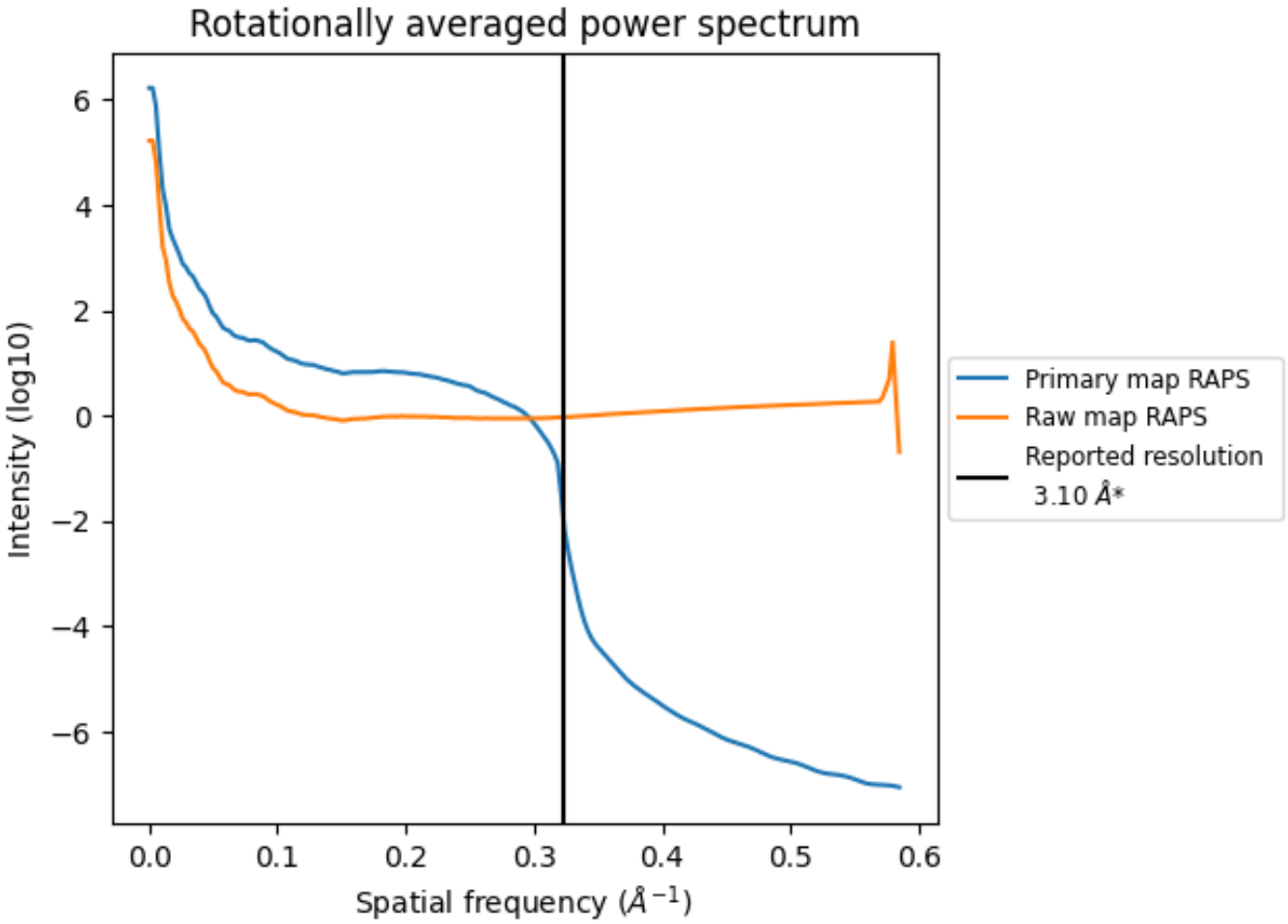
7.2 Volume estimate



The volume at the recommended contour level is 585 nm^3; this corresponds to an approximate mass of 529 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 (i)

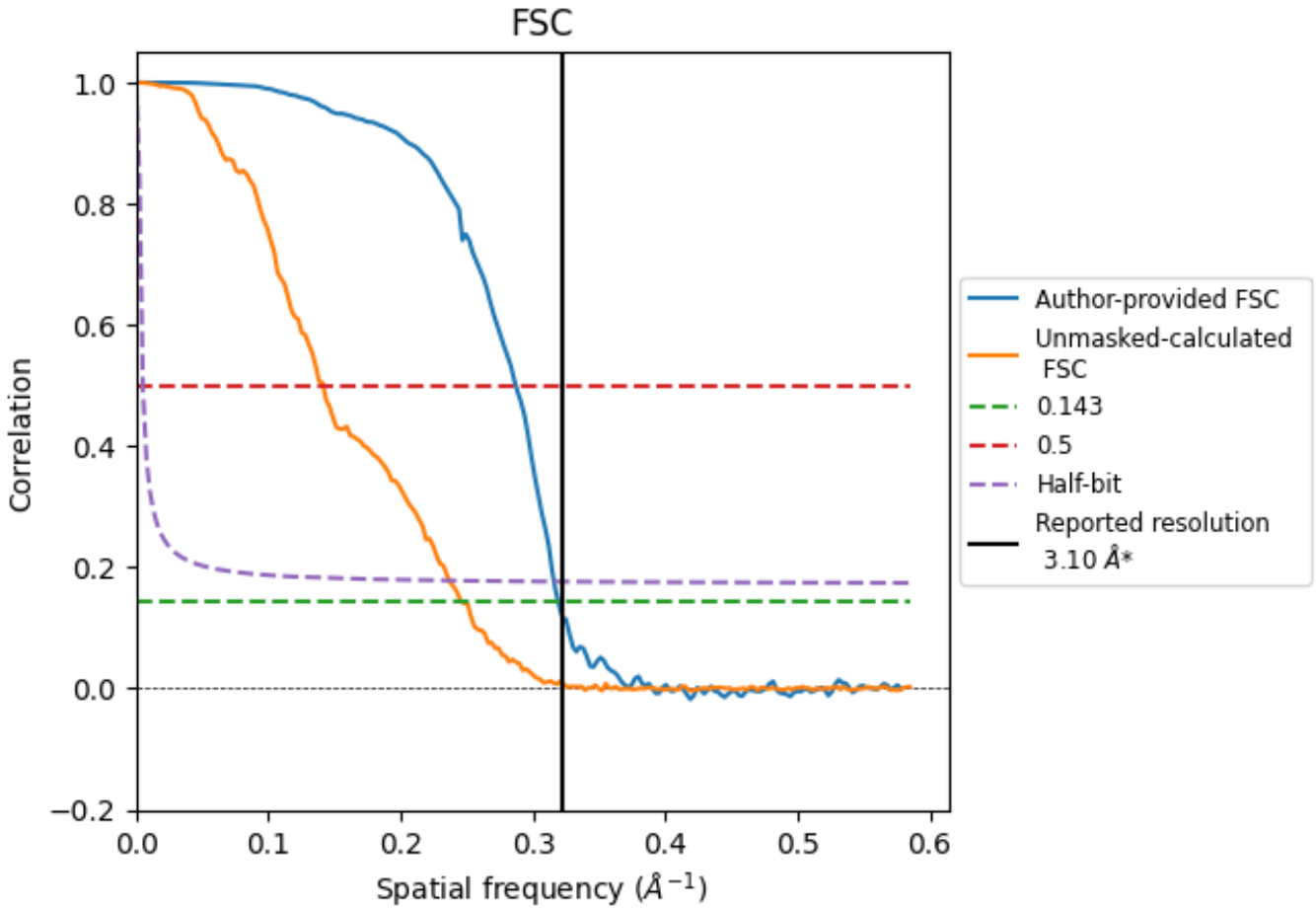


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

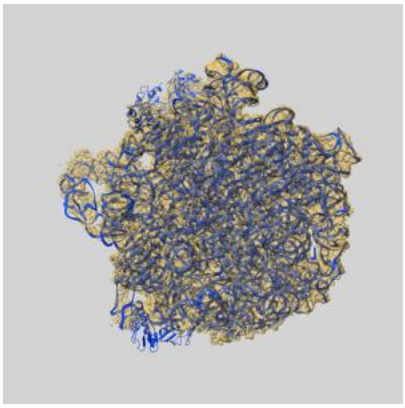
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.48	3.16
Unmasked-calculated*	4.06	7.07	4.22

*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 4.06 differs from the reported value 3.1 by more than 10 %

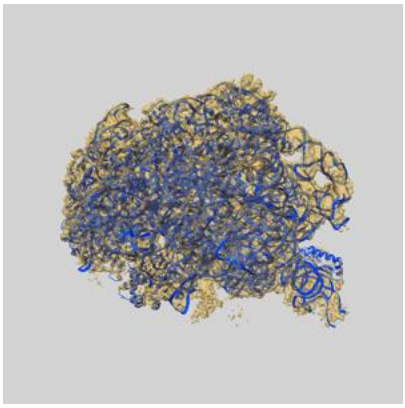
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44871 and PDB model 9BSS. Per-residue inclusion information can be found in section 3 on page 9.

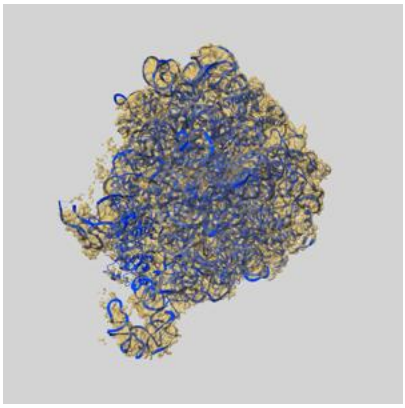
9.1 Map-model overlay



X



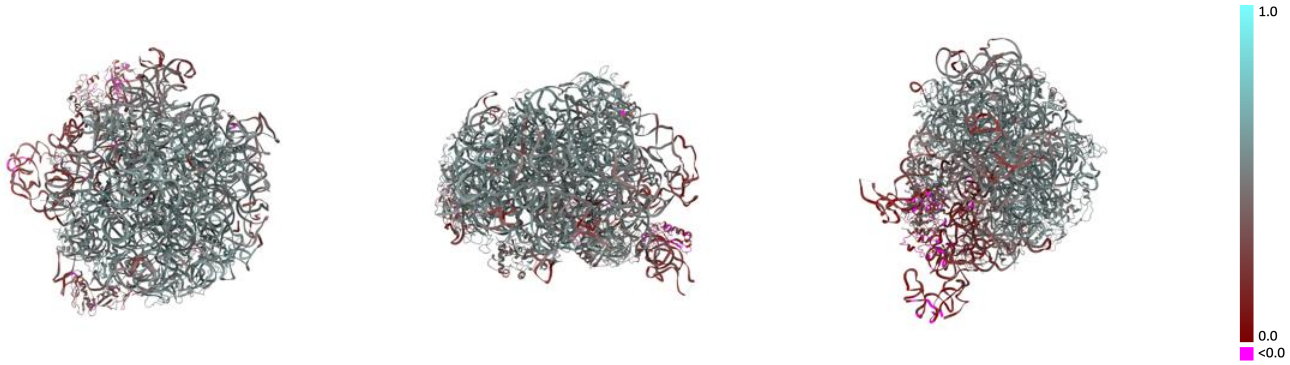
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.146 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.

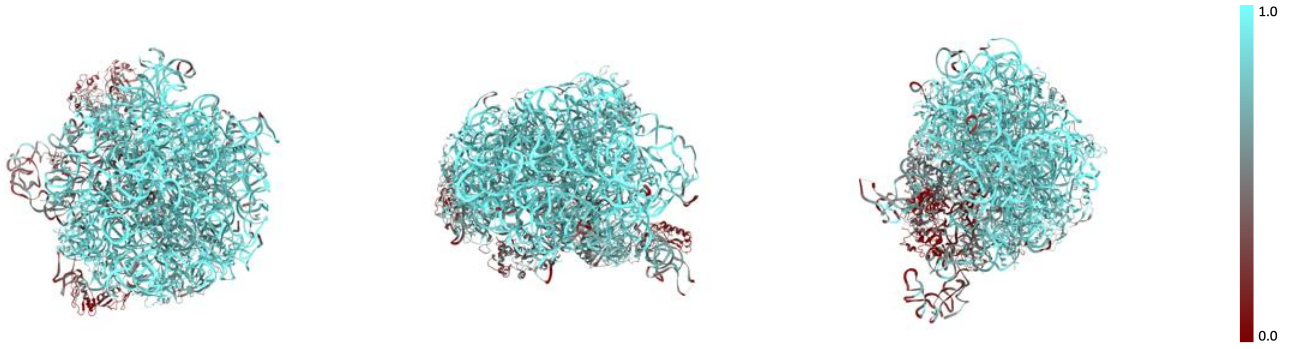
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

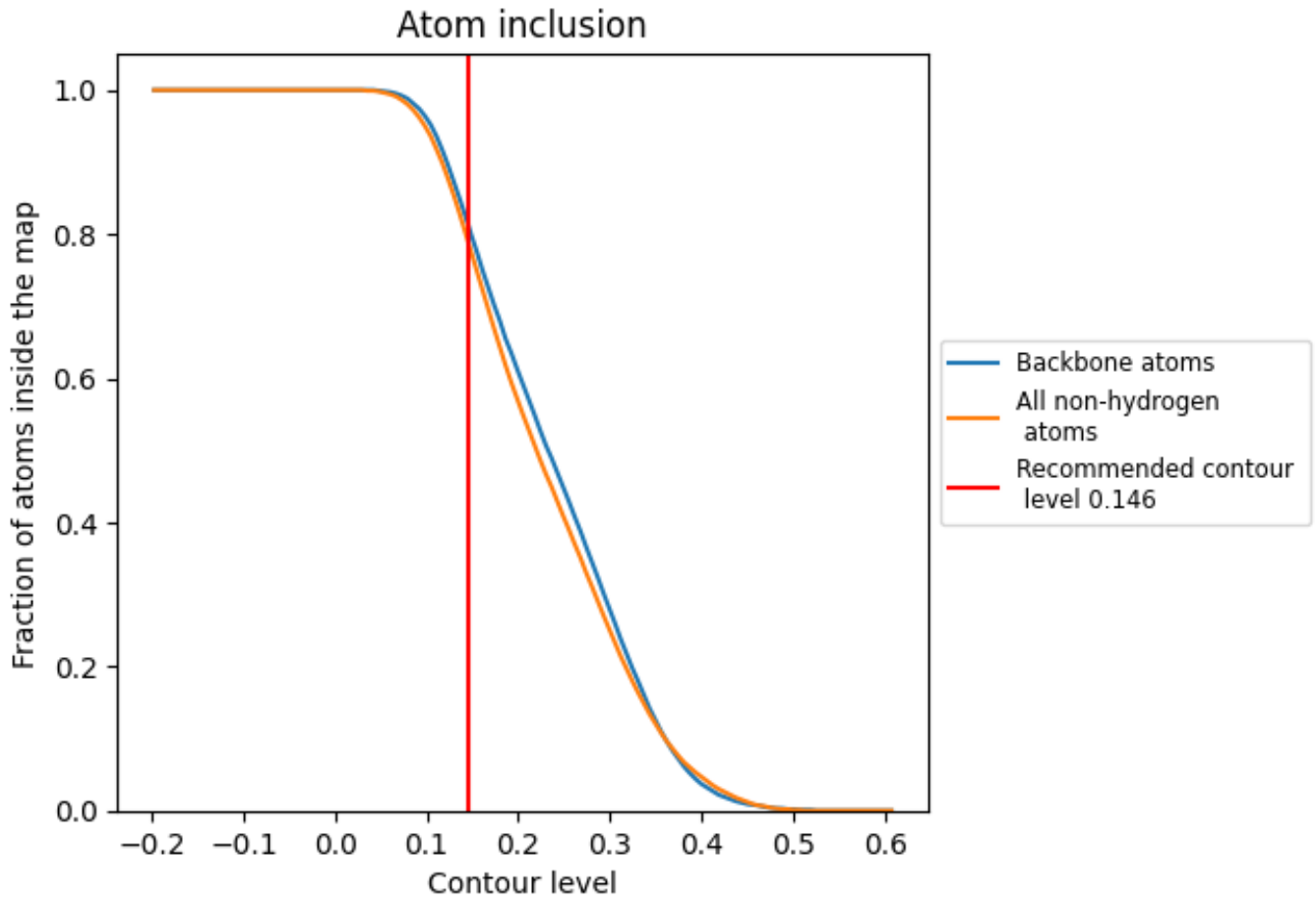
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.146).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.146) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7870	0.4560
A	0.8610	0.4600
B	0.3520	0.1720
C	0.8320	0.5530
D	0.8510	0.5590
E	0.7770	0.5270
F	0.1070	0.2950
G	0.8670	0.5510
H	0.7170	0.5390
I	0.6390	0.4490
J	0.8770	0.5590
K	0.7310	0.5440
L	0.8890	0.5490
M	0.8130	0.5460
N	0.8720	0.5610
O	0.8490	0.5360
P	0.7880	0.5230
Q	0.2130	0.3510
R	0.7920	0.4850
S	0.7620	0.5140
T	0.8150	0.4430
U	0.9250	0.5730
V	0.5150	0.4630
W	0.5250	0.4300
Y	0.0630	0.0950