



## Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 06:07 am GMT

PDB ID : 7ASM  
EMDB ID : EMD-11900  
Title : Staphylococcus aureus 50S after 30 minutes incubation at 37C  
Authors : Camicata, G.; Bashan, A.; Yonath, A.  
Deposited on : 2020-10-27  
Resolution : 2.48 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](mailto: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>.

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

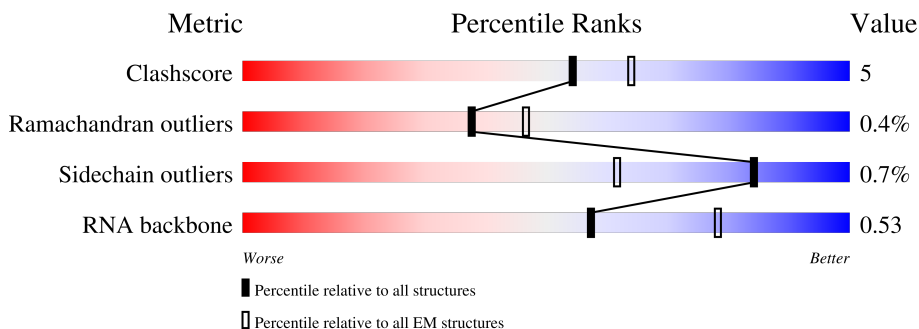
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.48 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	N	114	91% (green), 9% (yellow)
2	E	206	90% (green), 10% (yellow)
3	A	2923	66% (green), 25% (yellow), 6% (orange), 3% (red), 0% (grey)
4	B	115	57% (green), 38% (yellow), 5% (orange)
5	C	274	94% (green), 5% (yellow)
6	G	175	79% (green), 21% (yellow)
7	H	145	81% (green), 18% (yellow), 1% (orange)

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Mol	Chain	Length	Quality of chain
8	J	146	88% 12%
9	K	137	93% 7%
10	M	119	80% 19%
11	O	116	89% 10%
12	P	102	87% 12%
13	R	89	90% 10%
14	S	104	81% 15%
15	T	94	84% 16%
16	U	79	96%
17	W	67	97%
18	3	64	89% 11%
19	1	47	91% 9%
20	2	43	95% 5%
21	4	37	78% 19%
22	D	215	81% 18%
23	F	158	13% 97%
24	I	122	83% 17%
25	Q	112	90% 10%
26	V	49	82% 16%
27	X	58	90% 10%
28	Z	48	98%
29	L	120	88% 11%

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 86149 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	N	114	889	563	175	151	0	0

- Molecule 2 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	206	1572	986	288	296	2	0	0

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A	2834	60769	27128	11118	19689	2834	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	B	115	2448	1094	436	803	115	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	274	2094	1303	415	371	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	175	1263	791	240	229	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	145	1149	717	211	218	3	0	0

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	146	1086	674	214	197	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	137	1071	689	203	175	4	0	0

- Molecule 10 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	M	119	882	549	174	159	0	0

- Molecule 11 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	116	942	593	189	156	4	0	0

- Molecule 12 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	102	790	503	142	144	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	R	89	715	453	127	131	4	0	0

- Molecule 14 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	S	100	755	477	139	138	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	49	GLN	ARG	conflict	UNP A0A6K7SSC4

- Molecule 15 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	T	94	722	463	130	129	0	0

- Molecule 16 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	U	79	597	369	117	111	0	0

- Molecule 17 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	W	67	541	333	102	106	0	0

- Molecule 18 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	3	64	521	324	113	82	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	1	47	390	238	78	70	4	0	0

- Molecule 20 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 21 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

- Molecule 22 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 23 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	F	158	Total	C	N	O	0	0
			778	462	158	158		

- Molecule 24 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	112	Total	C	N	O	S	0	0
			854	534	164	153	3		

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	V	49	Total	C	N	O	0	0
			379	234	82	63		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
27	X	58	Total	C	N	O	0	0
			449	280	85	84		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	48	Total	C	N	O	S	0	0
			360	222	77	59	2		

- Molecule 29 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L	120	Total	C	N	O	S	0	0
			925	573	181	170	1		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

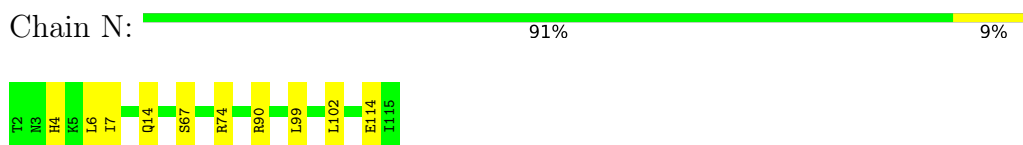
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Mg	0
			1	1	



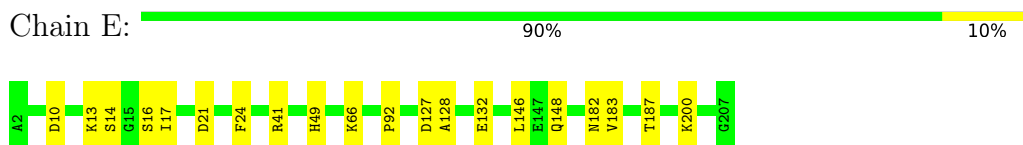
### 3 Residue-property plots

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

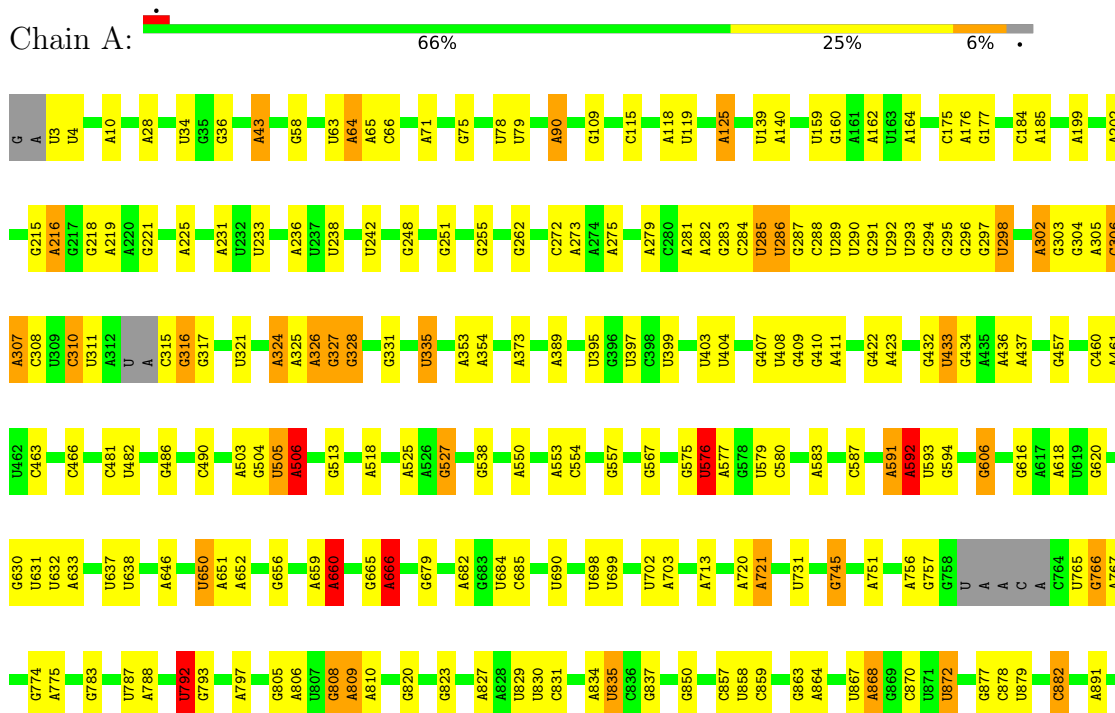
- Molecule 1: 50S ribosomal protein L19



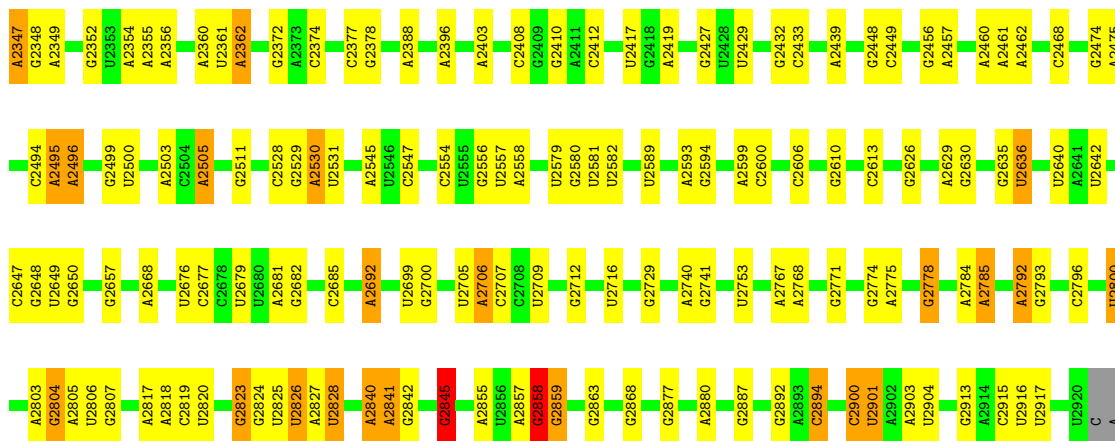
- Molecule 2: 50S ribosomal protein L4



- Molecule 3: 23S rRNA



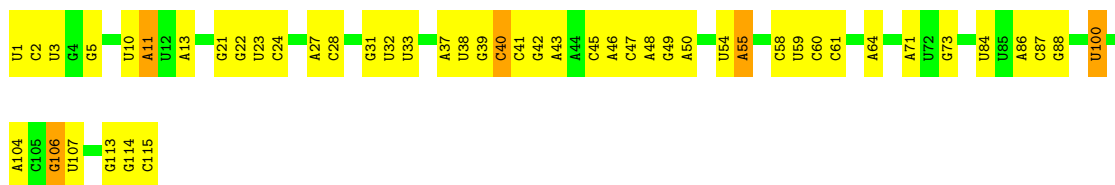




A

- Molecule 4: 5S rRNA

Chain B: 57% 38%



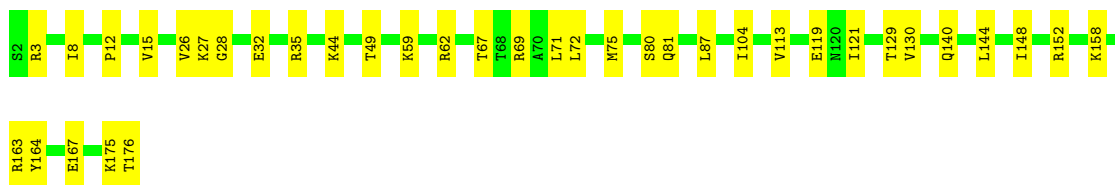
- Molecule 5: 50S ribosomal protein L2

Chain C: 94% 5%



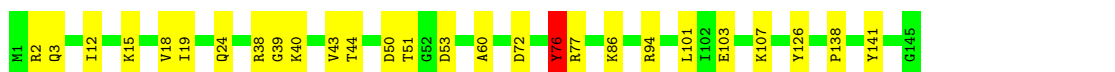
- Molecule 6: 50S ribosomal protein L6

Chain G: 79% 21%




- Molecule 7: 50S ribosomal protein L13

Chain H: 81% 18%



- Molecule 8: 50S ribosomal protein L15

Chain J:  88% 12%




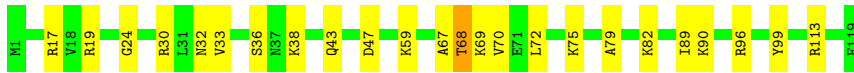
- Molecule 9: 50S ribosomal protein L16

Chain K:  93% 7%




- Molecule 10: 50S ribosomal protein L18

Chain M:  80% 19%




- Molecule 11: 50S ribosomal protein L20

Chain O:  89% 10%



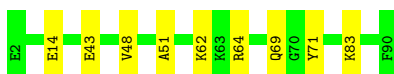
- Molecule 12: 50S ribosomal protein L21

Chain P:  87% 12%




- Molecule 13: 50S ribosomal protein L23

Chain R:  90% 10%




- Molecule 14: 50S ribosomal protein L24

Chain S:  81% 15%



- Molecule 15: 50S ribosomal protein L25

Chain T:  84% 16%



- Molecule 16: 50S ribosomal protein L27

Chain U:  96%




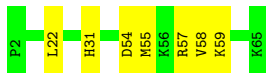
- Molecule 17: 50S ribosomal protein L29

Chain W:  97%




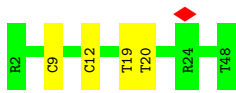
- Molecule 18: 50S ribosomal protein L35

Chain 3:  89% 11%



- Molecule 19: 50S ribosomal protein L33

Chain 1:  91% 9%




- Molecule 20: 50S ribosomal protein L34

Chain 2:  95% 5%




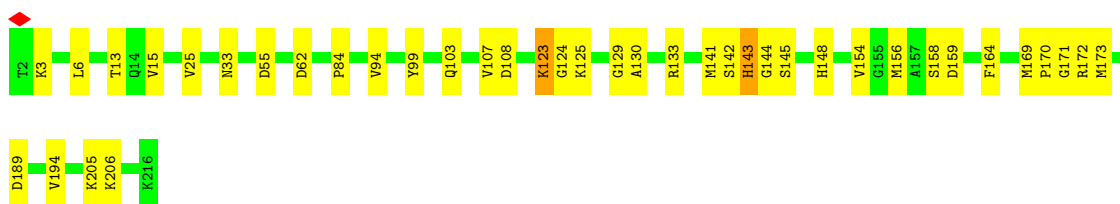
- Molecule 21: 50S ribosomal protein L36

Chain 4:  78% 19%



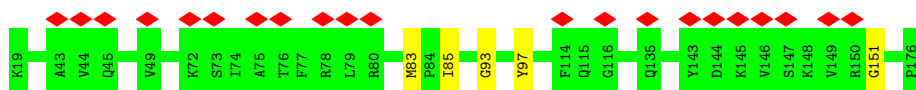
- Molecule 22: 50S ribosomal protein L3

Chain D:  81% 18%




- Molecule 23: 50S ribosomal protein L5

Chain F:  13% 97%




- Molecule 24: 50S ribosomal protein L14

Chain I:  83% 17%




- Molecule 25: 50S ribosomal protein L22

Chain Q:  90% 10%




- Molecule 26: 50S ribosomal protein L28

Chain V:  82% 16%



- Molecule 27: 50S ribosomal protein L30

Chain X:  90% 10%

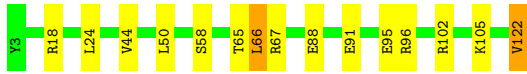
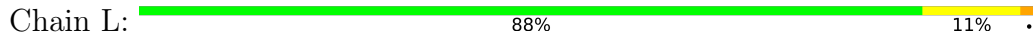


- Molecule 28: 50S ribosomal protein L32

Chain Z:  98%



- Molecule 29: 50S ribosomal protein L17



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0037	Depositor
Map size ( $\text{\AA}$ )	308.88, 308.88, 308.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.85800004, 0.85800004, 0.85800004	Depositor



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, 2MA

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	N	0.52	0/901	0.51	0/1209
2	E	0.51	0/1595	0.53	0/2154
3	A	1.18	16/67978 (0.0%)	0.96	112/106007 (0.1%)
4	B	0.73	0/2736	0.80	1/4261 (0.0%)
5	C	0.50	0/2129	0.52	0/2858
6	G	0.32	0/1281	0.48	0/1735
7	H	0.59	0/1171	0.61	1/1577 (0.1%)
8	J	0.50	0/1100	0.54	0/1467
9	K	0.52	0/1095	0.50	0/1472
10	M	0.37	0/891	0.50	0/1194
11	O	0.59	0/954	0.51	0/1264
12	P	0.58	0/800	0.56	0/1070
13	R	0.52	0/723	0.50	0/966
14	S	0.43	0/763	0.51	0/1018
15	T	0.40	0/730	0.48	0/981
16	U	0.59	0/603	0.52	0/802
17	W	0.44	0/542	0.48	0/722
18	3	0.47	0/526	0.50	0/690
19	1	0.29	0/395	0.43	0/530
20	2	0.60	0/371	0.67	1/484 (0.2%)
21	4	0.40	0/298	0.48	0/392
22	D	0.59	0/1651	0.67	0/2215
23	F	0.25	0/777	0.43	0/1079
24	I	0.50	0/925	0.54	0/1242
25	Q	0.53	0/862	0.57	0/1161
26	V	0.41	0/384	0.55	0/515
27	X	0.48	0/451	0.52	0/606
28	Z	0.50	0/366	0.53	0/489
29	L	0.53	0/929	0.61	0/1244
All	All	1.04	16/93927 (0.0%)	0.88	115/141404 (0.1%)

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
5	C	0	1
7	H	0	1
10	M	0	1
12	P	0	1
21	4	0	1
22	D	0	3
29	L	0	1
All	All	0	9

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	666	A	N9-C4	-7.23	1.33	1.37
3	A	1228	A	N9-C4	-6.71	1.33	1.37
3	A	650	U	C2-N3	-6.47	1.33	1.37
3	A	1228	A	N3-C4	-6.32	1.31	1.34
3	A	721	A	N9-C4	-6.18	1.34	1.37
3	A	1599	G	N3-C4	-6.03	1.31	1.35
3	A	2740	A	N9-C4	-6.00	1.34	1.37
3	A	1599	G	N9-C4	-5.95	1.33	1.38
3	A	666	A	N3-C4	-5.89	1.31	1.34
3	A	2845	G	N9-C4	-5.89	1.33	1.38
3	A	1816	A	N9-C4	-5.61	1.34	1.37
3	A	1032	A	N9-C4	-5.51	1.34	1.37
3	A	2845	G	N3-C4	-5.48	1.31	1.35
3	A	125	A	N9-C4	-5.12	1.34	1.37
3	A	721	A	N3-C4	-5.11	1.31	1.34
3	A	1599	G	C2-N3	-5.06	1.28	1.32

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	576	U	N3-C2-O2	-10.60	114.78	122.20
3	A	1599	G	N3-C2-N2	-10.00	112.90	119.90
3	A	1599	G	N3-C4-N9	-9.88	120.07	126.00
3	A	557	G	O4'-C1'-N9	8.93	115.35	108.20
3	A	2845	G	C2-N3-C4	-8.84	107.48	111.90
3	A	2636	U	C2-N1-C1'	8.84	128.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	125	A	N7-C8-N9	8.38	117.99	113.80
3	A	1395	G	C4-C5-N7	8.05	114.02	110.80
3	A	1228	A	C5-N7-C8	-8.04	99.88	103.90
3	A	125	A	C5-N7-C8	-7.95	99.93	103.90
3	A	2053	U	N3-C2-O2	-7.83	116.72	122.20
3	A	576	U	N1-C2-O2	7.82	128.27	122.80
3	A	1228	A	N7-C8-N9	7.69	117.64	113.80
3	A	2845	G	C5-N7-C8	-7.58	100.51	104.30
3	A	1227	U	N3-C2-O2	-7.57	116.90	122.20
3	A	1032	A	C5-N7-C8	-7.43	100.19	103.90
3	A	1228	A	C2-N3-C4	-7.40	106.90	110.60
3	A	592	A	N1-C6-N6	-7.30	114.22	118.60
3	A	1490	G	N9-C4-C5	-7.30	102.48	105.40
3	A	1804	U	N3-C2-O2	-7.26	117.12	122.20
3	A	721	A	C5-N7-C8	-7.25	100.28	103.90
3	A	721	A	C2-N3-C4	-7.18	107.01	110.60
3	A	1049	C	N3-C2-O2	-7.18	116.88	121.90
3	A	1816	A	C5-N7-C8	-7.04	100.38	103.90
3	A	1599	G	N3-C4-C5	7.01	132.11	128.60
20	2	17	HIS	C-N-CA	-7.00	107.59	122.30
3	A	2845	G	N3-C4-C5	6.90	132.05	128.60
3	A	2845	G	N3-C4-N9	-6.87	121.88	126.00
3	A	721	A	O4'-C1'-N9	6.84	113.67	108.20
3	A	1395	G	C5-N7-C8	-6.76	100.92	104.30
3	A	1032	A	N7-C8-N9	6.63	117.12	113.80
3	A	1032	A	O4'-C1'-N9	6.50	113.40	108.20
3	A	2249	G	O4'-C1'-N9	6.48	113.39	108.20
3	A	1816	A	C4-C5-N7	6.36	113.88	110.70
3	A	2845	G	N7-C8-N9	6.36	116.28	113.10
3	A	666	A	C5-N7-C8	-6.36	100.72	103.90
3	A	1395	G	C6-C5-N7	-6.34	126.60	130.40
3	A	1490	G	N1-C6-O6	6.33	123.70	119.90
3	A	1228	A	C8-N9-C4	-6.32	103.27	105.80
3	A	2636	U	C6-N1-C1'	-6.32	112.36	121.20
3	A	835	U	C2-N1-C1'	6.30	125.26	117.70
3	A	2210	C	N3-C2-O2	-6.29	117.50	121.90
3	A	650	U	N3-C2-O2	-6.25	117.82	122.20
3	A	2302	C	C6-N1-C2	-6.25	117.80	120.30
3	A	125	A	C8-N9-C4	-6.24	103.31	105.80
3	A	1490	G	C6-C5-N7	-6.22	126.67	130.40
3	A	504	G	O4'-C1'-N9	6.21	113.17	108.20
3	A	1490	G	C8-N9-C1'	-6.20	118.94	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1228	A	O4'-C1'-N9	6.18	113.14	108.20
3	A	721	A	N7-C8-N9	6.17	116.89	113.80
3	A	2210	C	N1-C2-O2	6.17	122.60	118.90
3	A	882	C	N3-C2-O2	-6.12	117.62	121.90
3	A	2858	G	O4'-C1'-N9	6.11	113.09	108.20
3	A	576	U	P-O3'-C3'	6.09	127.01	119.70
3	A	1599	G	N9-C4-C5	6.06	107.82	105.40
3	A	1351	C	C2-N1-C1'	6.04	125.44	118.80
3	A	2900	C	C6-N1-C2	-6.04	117.89	120.30
3	A	666	A	C2-N3-C4	-6.02	107.59	110.60
3	A	1816	A	O4'-C1'-N9	5.97	112.98	108.20
3	A	1395	G	O4'-C1'-N9	5.96	112.97	108.20
3	A	2800	U	N3-C2-O2	-5.96	118.03	122.20
3	A	2868	G	O4'-C1'-N9	5.93	112.94	108.20
3	A	1395	G	N7-C8-N9	5.93	116.06	113.10
3	A	593	U	N3-C2-O2	-5.88	118.08	122.20
7	H	76	TYR	N-CA-C	5.88	126.88	111.00
3	A	1387	C	C2-N1-C1'	5.86	125.24	118.80
3	A	576	U	C2-N1-C1'	5.83	124.69	117.70
3	A	506	A	C5-N7-C8	-5.79	101.00	103.90
3	A	1511	C	N1-C2-O2	-5.75	115.45	118.90
3	A	1801	C	N3-C2-O2	-5.73	117.89	121.90
3	A	660	A	C8-N9-C4	-5.71	103.52	105.80
3	A	125	A	C2-N3-C4	-5.69	107.75	110.60
3	A	2740	A	C2-N3-C4	-5.68	107.76	110.60
3	A	1378	U	N3-C2-O2	-5.64	118.25	122.20
3	A	2709	U	N3-C2-O2	-5.63	118.26	122.20
3	A	2845	G	C8-N9-C4	-5.62	104.15	106.40
3	A	1601	U	N3-C2-O2	-5.61	118.27	122.20
3	A	1395	G	C4-N9-C1'	5.59	133.77	126.50
3	A	2419	A	O4'-C1'-N9	5.58	112.66	108.20
3	A	2894	C	C2-N1-C1'	5.58	124.93	118.80
3	A	2321	C	C2-N1-C1'	5.57	124.92	118.80
3	A	1032	A	C4-C5-N7	5.55	113.48	110.70
3	A	1599	G	N1-C2-N2	5.54	121.19	116.20
3	A	1343	U	C2-N1-C1'	5.49	124.29	117.70
3	A	1599	G	C8-N9-C1'	5.47	134.11	127.00
3	A	2845	G	C4-C5-N7	5.46	112.98	110.80
3	A	2647	C	O5'-P-OP1	-5.46	100.79	105.70
3	A	2017	C	N1-C2-O2	-5.44	115.64	118.90
3	A	335	U	C5-C4-O4	-5.41	122.65	125.90
3	A	2053	U	C5-C4-O4	5.41	129.15	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	335	U	C2-N1-C1'	5.39	124.17	117.70
3	A	2017	C	C2-N3-C4	-5.38	117.21	119.90
3	A	506	A	N7-C8-N9	5.36	116.48	113.80
3	A	576	U	C6-N1-C2	-5.33	117.80	121.00
3	A	882	C	C2-N1-C1'	5.32	124.66	118.80
3	A	2858	G	N3-C4-N9	-5.32	122.81	126.00
3	A	1566	G	N3-C4-N9	-5.30	122.82	126.00
3	A	2419	A	C5-N7-C8	-5.30	101.25	103.90
3	A	2636	U	N1-C2-O2	5.29	126.50	122.80
3	A	1228	A	C5-C6-N1	-5.21	115.09	117.70
3	A	2094	G	N3-C4-C5	-5.21	126.00	128.60
3	A	2053	U	N1-C2-N3	5.20	118.02	114.90
3	A	1387	C	N3-C2-O2	-5.19	118.27	121.90
3	A	721	A	C4-C5-N7	5.18	113.29	110.70
3	A	666	A	N1-C6-N6	5.15	121.69	118.60
3	A	1049	C	N1-C2-O2	5.15	121.99	118.90
3	A	2419	A	C4-C5-N7	5.12	113.26	110.70
3	A	1562	C	N1-C2-O2	5.11	121.96	118.90
3	A	2894	C	N3-C2-O2	-5.10	118.33	121.90
3	A	2092	C	C6-N1-C2	-5.10	118.26	120.30
3	A	576	U	C5-C4-O4	5.07	128.94	125.90
3	A	2249	G	C4-C5-N7	5.07	112.83	110.80
4	B	100	U	C2-N1-C1'	5.05	123.76	117.70
3	A	660	A	N7-C8-N9	5.05	116.32	113.80
3	A	2249	G	C5-N7-C8	-5.03	101.78	104.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	4	11	CYS	Peptide
5	C	233	GLY	Peptide
22	D	123	LYS	Peptide
22	D	142	SER	Peptide
22	D	144	GLY	Peptide
7	H	76	TYR	Peptide
29	L	66	LEU	Peptide
10	M	68	THR	Peptide
12	P	50	ALA	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	N	889	0	937	7	0
2	E	1572	0	1619	14	0
3	A	60769	0	30546	501	0
4	B	2448	0	1239	35	0
5	C	2094	0	2205	11	0
6	G	1263	0	1232	25	0
7	H	1149	0	1145	17	0
8	J	1086	0	1125	10	0
9	K	1071	0	1123	7	0
10	M	882	0	900	19	0
11	O	942	0	1014	10	0
12	P	790	0	830	10	0
13	R	715	0	748	6	0
14	S	755	0	803	10	0
15	T	722	0	766	9	0
16	U	597	0	604	2	0
17	W	541	0	563	2	0
18	3	521	0	586	5	0
19	1	390	0	394	3	0
20	2	367	0	415	1	0
21	4	295	0	339	7	0
22	D	1627	0	1667	20	0
23	F	778	0	348	3	0
24	I	918	0	981	13	0
25	Q	854	0	914	8	0
26	V	379	0	400	6	0
27	X	449	0	491	4	0
28	Z	360	0	358	1	0
29	L	925	0	975	10	0
30	A	1	0	0	0	0
All	All	86149	0	55267	721	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (721) 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)
3:A:1521:A:N6	3:A:1559:G:H1	1.50	1.10
3:A:1514:A:N1	3:A:1566:G:N2	2.08	1.01
3:A:2128:G:H1	3:A:2215:U:H3	1.00	0.95
3:A:2127:G:H1	3:A:2216:U:H3	1.13	0.94
3:A:1578:A:N6	3:A:1591:G:N7	2.15	0.93
3:A:1521:A:N1	3:A:1559:G:N2	2.17	0.92
3:A:1484:G:H1	3:A:1599:G:H22	1.08	0.92
3:A:1514:A:H61	3:A:1566:G:H1	1.17	0.92
3:A:1450:A:N6	3:A:1634:A:N1	2.19	0.91
3:A:1489:A:O2'	3:A:1490:G:N7	2.01	0.90
3:A:316:G:H1	3:A:403:U:H3	0.98	0.90
3:A:2858:G:O2'	3:A:2859:G:N7	2.05	0.89
3:A:1515:G:H22	3:A:1565:U:H3	1.17	0.87
3:A:2863:G:H1	3:A:2894:C:H5	1.20	0.86
3:A:656:G:H21	3:A:660:A:H2	1.19	0.85
3:A:115:C:HO2'	3:A:125:A:H8	1.25	0.85
3:A:922:G:H1	3:A:945:A:H61	1.23	0.85
3:A:2432:G:H21	3:A:2439:A:H62	1.23	0.84
3:A:1387:C:H5	3:A:1418:G:H1	1.25	0.84
3:A:1484:G:H1	3:A:1599:G:N2	1.76	0.83
3:A:1862:G:H1	3:A:1932:C:H5	1.27	0.82
3:A:1522:G:H1	3:A:1558:U:H3	1.27	0.81
3:A:882:C:H5	3:A:986:G:H1	1.26	0.80
3:A:2125:U:O2	3:A:2218:G:N1	2.15	0.80
3:A:2649:U:O2'	3:A:2845:G:N2	2.15	0.80
3:A:1094:A:N6	3:A:1153:C:O2	2.14	0.80
2:E:182:ASN:HB3	3:A:660:A:H8	1.46	0.80
3:A:922:G:H1	3:A:945:A:N6	1.78	0.80
3:A:1757:U:O2	3:A:1772:G:N1	2.16	0.79
3:A:1767:G:OP1	3:A:1769:C:N4	2.15	0.79
3:A:275:A:H62	3:A:296:G:H21	1.30	0.79
3:A:1663:G:HO2'	20:2:2:VAL:N	1.82	0.78
3:A:1884:G:H21	3:A:1912:A:H62	1.32	0.78
3:A:2140:C:N4	3:A:2196:G:N7	2.33	0.77
3:A:2857:A:H3'	3:A:2858:G:H8	1.49	0.77
26:V:58:LYS:NZ	26:V:59:VAL:O	2.18	0.76
3:A:1189:C:O2'	3:A:1190:A:O5'	2.02	0.76
3:A:1579:C:H3'	3:A:1581:U:H3	1.50	0.75
3:A:2857:A:H3'	3:A:2858:G:C8	2.22	0.75
3:A:986:G:HO2'	3:A:1228:A:H8	1.35	0.75
22:D:3:LYS:HB3	22:D:94:VAL:HG12	1.70	0.74
14:S:3:ILE:HD11	14:S:33:VAL:HG11	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:606:G:OP2	12:P:78:ARG:NH2	2.20	0.74
3:A:1493:U:O2	3:A:1505:G:N2	2.20	0.74
3:A:2127:G:N2	3:A:2216:U:O2	2.20	0.73
3:A:1521:A:H61	3:A:1559:G:H1	0.77	0.73
3:A:275:A:H62	3:A:296:G:N2	1.86	0.72
1:N:74:ARG:HD3	24:I:77:ILE:HD13	1.71	0.72
3:A:162:A:H8	3:A:2244:G:H21	1.37	0.72
3:A:1770:C:N4	3:A:1771:A:N3	2.37	0.72
18:3:54:ASP:OD1	18:3:57:ARG:NH1	2.23	0.72
9:K:30:GLY:O	9:K:134:ARG:NH1	2.23	0.72
19:1:19:THR:HG22	19:1:20:THR:H	1.55	0.72
3:A:1902:G:H21	3:A:1903:A:H1'	1.52	0.71
3:A:1487:G:H22	3:A:1596:G:N2	1.87	0.71
3:A:1757:U:O4	3:A:1771:A:N6	2.24	0.71
3:A:326:A:H1'	3:A:327:G:H5'	1.73	0.71
3:A:1487:G:H22	3:A:1596:G:H22	1.37	0.71
3:A:2432:G:N2	3:A:2439:A:H62	1.87	0.71
3:A:1218:G:H2'	3:A:1219:G:C8	2.26	0.70
3:A:1493:U:H3	3:A:1505:G:H1	1.37	0.70
3:A:2136:U:O2'	3:A:2169:G:O2'	2.09	0.70
3:A:1049:C:H5	3:A:1182:G:H1	1.39	0.70
29:L:24:LEU:HD23	29:L:44:VAL:HG21	1.72	0.70
3:A:1487:G:H1	3:A:1596:G:H1	1.38	0.69
3:A:315:C:O2'	3:A:316:G:N7	2.21	0.69
3:A:2606:C:O2'	22:D:145:SER:O	2.10	0.69
3:A:591:A:H4'	3:A:592:A:H5'	1.73	0.69
3:A:2195:G:N2	3:A:2197:G:O6	2.26	0.69
3:A:721:A:H8	3:A:2096:G:H21	1.41	0.69
10:M:96:ARG:NH2	10:M:99:TYR:O	2.27	0.68
3:A:284:C:HO2'	3:A:287:G:H1	0.70	0.67
3:A:1458:A:N1	3:A:1459:A:N6	2.42	0.67
3:A:2162:A:H62	3:A:2183:G:H21	1.40	0.67
3:A:923:A:H2	3:A:944:G:H22	1.41	0.67
3:A:1760:G:H1	3:A:1768:C:H42	1.42	0.67
21:4:11:CYS:HB2	21:4:14:CYS:H	1.60	0.67
3:A:1463:A:N7	3:A:1625:U:O2	2.28	0.67
7:H:39:GLY:HA3	7:H:51:THR:HG23	1.77	0.67
21:4:11:CYS:SG	21:4:32:HIS:ND1	2.60	0.67
3:A:2901:U:OP1	29:L:96:ARG:NH2	2.27	0.66
3:A:1036:C:H2'	3:A:1037:A:H5''	1.77	0.66
3:A:1633:A:H2'	3:A:1634:A:C8	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1219:G:H2'	3:A:1220:A:C8	2.30	0.66
3:A:1552:U:O2'	3:A:1553:A:O4'	2.14	0.66
3:A:1947:C:H2'	3:A:1948:G:H8	1.60	0.66
14:S:97:SER:OG	14:S:98:GLY:N	2.28	0.66
3:A:2216:U:H2'	3:A:2217:G:C8	2.31	0.66
14:S:79:THR:OG1	14:S:94:ALA:O	2.12	0.66
22:D:6:LEU:H	22:D:33:ASN:HD21	1.42	0.66
3:A:1760:G:H3'	3:A:1761:G:H4'	1.77	0.66
3:A:1488:A:H3'	3:A:1489:A:H8	1.60	0.65
3:A:1915:G:N2	3:A:1915:G:OP2	2.28	0.65
3:A:1218:G:H2'	3:A:1219:G:H8	1.62	0.65
3:A:1631:G:N2	3:A:1631:G:OP1	2.28	0.65
3:A:2840:A:O2'	3:A:2841:A:OP1	2.14	0.65
5:C:10:THR:HG22	5:C:12:GLY:H	1.59	0.65
3:A:1579:C:H5	3:A:1586:U:H3	1.44	0.65
3:A:1628:A:H2'	3:A:1629:U:C6	2.31	0.65
3:A:1598:U:H2'	3:A:1599:G:C8	2.32	0.65
3:A:2208:A:N6	3:A:2209:G:O6	2.30	0.64
3:A:1884:G:N2	3:A:1912:A:H62	1.94	0.64
3:A:2554:C:H5''	21:4:30:PRO:HB2	1.78	0.64
3:A:139:U:O2	3:A:1446:U:O2'	2.13	0.64
27:X:12:VAL:HG22	27:X:20:ARG:HG2	1.80	0.64
3:A:1893:A:H62	3:A:1903:A:H62	1.46	0.64
3:A:2778:G:OP1	6:G:3:ARG:NH2	2.31	0.63
3:A:927:G:OP2	3:A:927:G:N2	2.32	0.63
3:A:1512:U:H2'	3:A:1513:A:C8	2.33	0.63
1:N:67:SER:OG	24:I:120:GLU:OE2	2.17	0.63
3:A:921:C:H42	3:A:946:A:H61	1.46	0.63
3:A:1769:C:N3	3:A:1770:C:N4	2.47	0.62
3:A:1946:A:H2'	3:A:1947:C:C6	2.34	0.62
3:A:1487:G:N2	3:A:1596:G:H22	1.97	0.62
6:G:164:TYR:HB2	6:G:167:GLU:HB2	1.81	0.62
3:A:870:C:O2'	8:J:54:GLN:NE2	2.26	0.62
3:A:1478:A:H61	3:A:1605:A:N6	1.97	0.62
3:A:288:C:H2'	3:A:289:U:C6	2.35	0.62
25:Q:25:ARG:NH1	25:Q:74:ALA:O	2.32	0.62
21:4:11:CYS:HB2	21:4:14:CYS:N	2.15	0.61
14:S:47:PRO:HB3	14:S:53:GLU:HA	1.81	0.61
3:A:1057:A:HO2'	3:A:1058:U:H6	1.48	0.61
3:A:288:C:H2'	3:A:289:U:H6	1.65	0.61
3:A:2146:A:H2'	3:A:2147:G:H5''	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1453:G:H4'	3:A:1631:G:H22	1.66	0.61
3:A:2178:U:H2'	3:A:2179:A:C8	2.36	0.61
3:A:2340:C:H2'	3:A:2341:A:H8	1.66	0.61
3:A:943:C:H2'	3:A:944:G:C8	2.35	0.60
3:A:1582:U:O2	3:A:1586:U:O2'	2.16	0.60
3:A:1343:U:H5	3:A:1666:A:N1	1.99	0.60
3:A:1804:U:H5	3:A:1814:A:N1	1.98	0.60
3:A:1582:U:O4	3:A:1587:C:O2'	2.19	0.60
3:A:1569:G:N2	3:A:1569:G:OP1	2.34	0.60
3:A:2135:U:OP2	3:A:2205:C:N4	2.34	0.60
3:A:2150:A:N6	3:A:2199:U:OP1	2.34	0.60
3:A:1767:G:P	3:A:1768:C:H41	2.24	0.60
3:A:1759:G:H2'	3:A:1760:G:H8	1.65	0.60
4:B:38:U:O2'	4:B:43:A:N6	2.34	0.60
21:4:16:VAL:HG22	21:4:25:VAL:HG12	1.84	0.60
3:A:2138:U:O2'	3:A:2172:C:N4	2.35	0.60
13:R:51:ALA:HB2	13:R:83:LYS:HG3	1.83	0.60
3:A:867:U:H2'	3:A:868:A:H5''	1.83	0.60
3:A:922:G:N2	3:A:945:A:N1	2.44	0.60
3:A:928:C:N4	3:A:938:G:OP2	2.35	0.59
3:A:316:G:N2	3:A:403:U:O2	2.30	0.59
3:A:353:A:O2'	3:A:354:A:O5'	2.19	0.59
3:A:1595:C:H2'	3:A:1596:G:C8	2.37	0.59
6:G:59:LYS:HA	6:G:62:ARG:HG2	1.84	0.59
3:A:281:A:H2'	3:A:282:A:C8	2.38	0.59
3:A:2331:G:H22	3:A:2339:U:H3	1.50	0.59
3:A:175:C:H2'	3:A:176:A:O4'	2.03	0.58
3:A:1847:U:H5	5:C:177:ARG:HH21	1.50	0.58
8:J:19:VAL:HG23	8:J:27:ASN:HB3	1.84	0.58
3:A:1185:U:H4'	3:A:1186:A:O4'	2.02	0.58
3:A:1759:G:H2'	3:A:1760:G:C8	2.39	0.58
4:B:27:A:H2'	4:B:28:C:C6	2.39	0.58
3:A:788:A:O2'	3:A:1703:U:OP1	2.21	0.58
7:H:18:VAL:HG23	7:H:138:PRO:HB2	1.86	0.58
3:A:1630:A:H3'	3:A:1631:G:H5''	1.84	0.58
3:A:410:G:H4'	3:A:411:A:H5'	1.86	0.58
3:A:1449:A:H62	3:A:1634:A:H62	1.52	0.58
3:A:1897:U:H4'	3:A:1898:C:H5''	1.85	0.58
3:A:2432:G:H21	3:A:2439:A:N6	2.00	0.58
3:A:1453:G:H4'	3:A:1455:U:H3	1.66	0.57
3:A:1758:A:H1'	3:A:1772:G:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2216:U:H2'	3:A:2217:G:H8	1.69	0.57
3:A:1823:U:H2'	3:A:1824:C:C6	2.39	0.57
3:A:2355:A:H2'	3:A:2356:A:C8	2.39	0.57
3:A:684:U:H2'	3:A:685:C:C6	2.39	0.57
3:A:765:U:O2'	3:A:766:G:H8	1.87	0.57
2:E:127:ASP:OD1	2:E:128:ALA:N	2.37	0.57
3:A:1893:A:N6	3:A:1903:A:H62	2.02	0.57
3:A:2186:G:H2'	3:A:2187:G:C8	2.40	0.57
3:A:115:C:O2'	3:A:125:A:H8	1.84	0.57
3:A:1586:U:H2'	3:A:1587:C:O4'	2.04	0.57
22:D:189:ASP:HB3	22:D:194:VAL:HG22	1.87	0.57
24:I:6:THR:O	24:I:21:THR:HG22	2.04	0.57
29:L:95:GLU:N	29:L:95:GLU:OE1	2.38	0.57
3:A:579:U:H5'	11:O:42:SER:HB2	1.85	0.57
3:A:1756:U:H2'	3:A:1757:U:O4'	2.05	0.57
3:A:2149:U:H2'	3:A:2150:A:C8	2.39	0.57
3:A:2360:A:H5'	3:A:2362:A:H1'	1.86	0.57
6:G:87:LEU:HD21	6:G:148:ILE:HD11	1.86	0.57
3:A:1151:G:H2'	3:A:1152:U:C6	2.40	0.57
3:A:1627:G:H2'	3:A:1628:A:C8	2.40	0.56
3:A:2511:G:OP1	9:K:45:ARG:NH2	2.38	0.56
4:B:54:U:H4'	4:B:55:A:H5'	1.87	0.56
3:A:302:A:H2'	3:A:303:G:C8	2.39	0.56
3:A:1806:U:H5	3:A:1811:A:N7	2.02	0.56
8:J:79:LEU:HB2	8:J:113:GLY:HA2	1.88	0.56
26:V:27:ARG:NH1	26:V:28:ARG:O	2.38	0.56
3:A:1160:C:H2'	3:A:1161:A:H8	1.70	0.56
22:D:141:MET:HE1	22:D:148:HIS:HB3	1.87	0.56
3:A:221:G:H22	3:A:238:U:H4'	1.70	0.56
3:A:1489:A:H2	3:A:1508:C:N4	2.04	0.56
3:A:1829:A:H2'	3:A:1830:A:C8	2.41	0.56
3:A:2845:G:O5'	3:A:2845:G:H8	1.88	0.56
3:A:1494:G:H1	3:A:1504:U:H3	1.52	0.56
3:A:2125:U:H2'	3:A:2126:C:C6	2.41	0.56
2:E:132:GLU:OE1	2:E:132:GLU:N	2.33	0.56
3:A:1456:U:H2'	3:A:1457:U:O4'	2.05	0.56
3:A:2347:A:HO2'	3:A:2349:A:H62	1.52	0.55
6:G:72:LEU:HA	6:G:75:MET:HG2	1.87	0.55
3:A:1917:A:H3'	3:A:1918:G:H8	1.70	0.55
29:L:65:THR:HG22	29:L:66:LEU:H	1.71	0.55
3:A:2128:G:N2	3:A:2215:U:O2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2219:C:H2'	3:A:2220:U:C6	2.41	0.55
6:G:15:VAL:HG22	6:G:28:GLY:HA3	1.89	0.55
3:A:159:U:H2'	3:A:160:G:C8	2.42	0.55
3:A:2313:A:H4'	3:A:2314:A:O4'	2.06	0.55
22:D:143:HIS:H	22:D:143:HIS:CD2	2.25	0.55
1:N:14:GLN:HE22	22:D:15:VAL:HG13	1.72	0.55
2:E:182:ASN:HB3	3:A:660:A:C8	2.35	0.55
3:A:302:A:H2'	3:A:303:G:H8	1.71	0.55
3:A:2079:G:H4'	22:D:156:MET:O	2.07	0.55
7:H:43:VAL:O	7:H:44:THR:OG1	2.17	0.55
12:P:56:ALA:HA	12:P:101:ASN:O	2.07	0.55
3:A:631:U:H2'	3:A:632:U:C6	2.42	0.54
4:B:32:U:O2'	4:B:42:G:N7	2.31	0.54
3:A:1450:A:H5''	3:A:1451:U:H5	1.73	0.54
15:T:72:VAL:HG21	15:T:91:PHE:HB3	1.88	0.54
3:A:316:G:O6	3:A:403:U:O4	2.26	0.54
12:P:1:MET:SD	12:P:1:MET:N	2.78	0.54
3:A:1631:G:H1'	3:A:1632:A:C8	2.42	0.54
3:A:2558:A:N7	6:G:176:THR:HA	2.22	0.54
3:A:1085:U:H3	3:A:1158:G:H1	1.55	0.54
3:A:2343:U:H2'	3:A:2344:C:C6	2.43	0.54
3:A:651:A:H2'	3:A:652:A:C8	2.43	0.54
3:A:1487:G:H1	3:A:1596:G:H22	1.55	0.54
14:S:22:LYS:H	14:S:36:GLU:HG2	1.73	0.54
3:A:1959:A:H2'	3:A:1960:G:O4'	2.08	0.54
3:A:2685:C:OP1	6:G:158:LYS:NZ	2.39	0.54
22:D:62:ASP:OD1	22:D:62:ASP:N	2.41	0.53
3:A:2318:U:H2'	3:A:2319:U:C6	2.43	0.53
7:H:72:ASP:OD1	7:H:72:ASP:N	2.35	0.53
3:A:1520:A:C6	3:A:1561:G:C4	2.97	0.53
3:A:1635:A:H2'	3:A:1636:U:C6	2.44	0.53
5:C:121:GLU:OE1	5:C:121:GLU:N	2.37	0.53
3:A:2682:G:N2	3:A:2692:A:OP2	2.37	0.53
24:I:19:VAL:HG22	24:I:41:CYS:HB2	1.90	0.53
4:B:113:G:H2'	4:B:114:G:O4'	2.09	0.53
6:G:129:THR:HG23	6:G:130:VAL:HG23	1.91	0.53
3:A:407:G:H2'	3:A:408:U:C6	2.44	0.53
3:A:1463:A:N7	3:A:1625:U:C2	2.77	0.53
3:A:1482:U:H3	3:A:1601:U:H5	1.56	0.53
3:A:2325:A:N6	3:A:2345:A:O2'	2.42	0.53
3:A:1053:A:OP1	7:H:40:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:69:LYS:HA	10:M:72:LEU:HD12	1.91	0.53
3:A:2824:G:H2'	3:A:2825:U:C6	2.43	0.52
3:A:2448:G:N7	18:3:31:HIS:NE2	2.57	0.52
15:T:71:LYS:HB3	15:T:94:ILE:HD11	1.91	0.52
3:A:579:U:H2'	3:A:580:C:C6	2.44	0.52
3:A:2124:U:H2'	3:A:2125:U:O4'	2.10	0.52
25:Q:11:ARG:O	25:Q:11:ARG:HG3	2.08	0.52
3:A:327:G:O2'	3:A:328:G:H5''	2.09	0.52
3:A:1757:U:H3'	3:A:1758:A:H8	1.75	0.52
14:S:45:GLN:HE22	14:S:57:LEU:HB2	1.73	0.52
3:A:289:U:H2'	3:A:290:U:C6	2.45	0.52
3:A:1510:U:H3	3:A:1571:G:H1	1.58	0.52
4:B:11:A:O2'	4:B:13:A:OP2	2.24	0.52
10:M:24:GLY:N	10:M:47:ASP:OD2	2.27	0.52
13:R:64:ARG:HE	13:R:69:GLN:HA	1.74	0.52
3:A:1501:G:H22	3:A:2729:G:H22	1.58	0.52
4:B:21:G:H2'	4:B:22:G:C8	2.45	0.52
2:E:16:SER:OG	2:E:17:ILE:N	2.42	0.52
3:A:316:G:H2'	3:A:317:G:C8	2.44	0.52
3:A:858:U:H2'	3:A:859:C:C6	2.45	0.52
3:A:290:U:H2'	3:A:291:G:H8	1.73	0.52
3:A:1219:G:H2'	3:A:1220:A:H8	1.72	0.52
3:A:285:U:O2'	3:A:286:U:H5''	2.09	0.52
3:A:632:U:H2'	3:A:633:A:C8	2.46	0.52
3:A:2140:C:N3	3:A:2195:G:O2'	2.34	0.52
3:A:864:A:N7	3:A:1227:U:H5	2.08	0.51
29:L:102:ARG:HH21	29:L:122:VAL:HB	1.75	0.51
3:A:2347:A:O2'	3:A:2349:A:N6	2.36	0.51
3:A:2668:A:N1	3:A:2800:U:H5	2.07	0.51
3:A:433:U:H5'	3:A:434:G:C2	2.45	0.51
3:A:1051:C:OP1	7:H:38:ARG:NH1	2.43	0.51
3:A:1507:A:H2'	3:A:1508:C:C6	2.45	0.51
3:A:1907:U:H2'	3:A:1908:A:C8	2.45	0.51
3:A:921:C:H42	3:A:946:A:N6	2.07	0.51
3:A:2037:G:H5''	25:Q:42:ALA:HB2	1.92	0.51
22:D:205:LYS:O	22:D:206:LYS:HG2	2.10	0.51
3:A:2705:U:O2'	3:A:2706:A:H8	1.92	0.51
4:B:5:G:H21	10:M:43:GLN:HE22	1.57	0.51
3:A:1456:U:OP2	3:A:1629:U:H5	1.93	0.51
2:E:17:ILE:HD11	2:E:200:LYS:HD3	1.93	0.51
3:A:64:A:H61	3:A:90:A:H62	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1160:C:H2'	3:A:1161:A:C8	2.46	0.50
3:A:1488:A:H3'	3:A:1489:A:C8	2.42	0.50
3:A:2313:A:H61	19:1:19:THR:HG21	1.74	0.50
3:A:115:C:O2'	3:A:125:A:C8	2.60	0.50
3:A:327:G:N2	3:A:399:U:O2	2.43	0.50
3:A:576:U:H2'	3:A:576:U:O2	2.09	0.50
23:F:83:MET:O	23:F:85:ILE:N	2.44	0.50
3:A:2676:U:H2'	3:A:2677:C:H6	1.76	0.50
3:A:2210:C:H2'	3:A:2211:U:C6	2.47	0.50
11:O:107:ALA:O	11:O:111:THR:HG23	2.12	0.50
3:A:921:C:N4	3:A:946:A:H61	2.07	0.50
10:M:30:ARG:NH1	10:M:32:ASN:HD22	2.10	0.50
3:A:1555:G:O2'	3:A:1556:G:N7	2.29	0.50
3:A:2326:G:H2'	3:A:2327:A:H8	1.76	0.50
3:A:1456:U:H3'	3:A:1457:U:C6	2.47	0.50
3:A:1488:A:H61	3:A:1595:C:H42	1.59	0.50
3:A:2162:A:H62	3:A:2183:G:N2	2.09	0.50
3:A:2824:G:H2'	3:A:2825:U:H6	1.77	0.50
3:A:868:A:H62	3:A:879:U:H3	1.60	0.50
7:H:94:ARG:HB3	7:H:101:LEU:HD22	1.93	0.50
3:A:1089:C:H4'	3:A:1091:G:H1'	1.94	0.50
3:A:221:G:N2	3:A:238:U:H4'	2.26	0.49
3:A:407:G:H2'	3:A:408:U:H6	1.77	0.49
3:A:2179:A:H2'	3:A:2180:C:C6	2.46	0.49
3:A:2273:G:H2'	3:A:2274:A:C8	2.47	0.49
3:A:2086:A:H2'	3:A:2530:2MA:HM23	1.94	0.49
3:A:2494:C:H2'	3:A:2495:A:O4'	2.13	0.49
24:I:77:ILE:O	24:I:77:ILE:HG13	2.12	0.49
3:A:896:U:H2'	3:A:897:A:H8	1.77	0.49
3:A:2053:U:H5	3:A:2064:A:N1	2.10	0.49
3:A:2180:C:H2'	3:A:2181:G:H8	1.77	0.49
3:A:306:C:H2'	3:A:307:A:H8	1.77	0.49
3:A:863:G:H21	3:A:1228:A:H2	1.60	0.49
3:A:922:G:H2'	3:A:923:A:C8	2.47	0.49
3:A:2152:G:O2'	3:A:2200:A:N6	2.41	0.49
3:A:2189:G:H21	3:A:2190:C:H41	1.61	0.49
10:M:67:ALA:HB3	10:M:72:LEU:HG	1.94	0.49
3:A:1158:G:H2'	3:A:1159:A:C8	2.47	0.49
3:A:1635:A:H2'	3:A:1636:U:H6	1.76	0.49
3:A:2155:C:H2'	3:A:2156:C:C6	2.48	0.49
9:K:43:THR:HG22	9:K:46:GLN:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:I:70:ARG:HB2	24:I:76:TYR:CE2	2.47	0.49
3:A:262:G:H21	3:A:666:A:H8	1.60	0.49
3:A:2403:A:N3	10:M:113:ARG:NH2	2.59	0.49
10:M:30:ARG:HH12	10:M:32:ASN:HD22	1.60	0.49
22:D:129:GLY:HA3	22:D:170:PRO:HA	1.93	0.49
1:N:4:HIS:HD2	1:N:6:LEU:H	1.60	0.49
3:A:294:G:H2'	3:A:295:G:H8	1.78	0.49
3:A:353:A:O2'	3:A:354:A:H2'	2.13	0.49
3:A:2141:A:H2'	3:A:2141:A:N3	2.27	0.49
3:A:2372:G:N3	3:A:2408:C:H2'	2.27	0.49
6:G:80:SER:OG	6:G:81:GLN:N	2.45	0.49
3:A:926:G:H3'	3:A:927:G:H21	1.78	0.49
3:A:1449:A:N6	3:A:1634:A:H62	2.11	0.49
3:A:1484:G:H22	3:A:1599:G:N2	2.11	0.49
3:A:2091:C:H2'	3:A:2092:C:C6	2.48	0.49
3:A:2499:G:H21	3:A:2505:A:H62	1.60	0.49
25:Q:11:ARG:HH11	25:Q:98:LYS:HD2	1.78	0.49
3:A:43:A:H62	3:A:482:U:H3	1.61	0.49
3:A:903:G:OP2	16:U:85:LYS:NZ	2.43	0.49
3:A:941:A:H2'	3:A:942:C:O4'	2.12	0.49
3:A:1903:A:N7	3:A:1904:A:C8	2.81	0.49
3:A:1847:U:C2	5:C:201:GLU:HG2	2.48	0.48
3:A:316:G:H2'	3:A:317:G:H8	1.78	0.48
3:A:702:U:H2'	3:A:703:A:C8	2.48	0.48
3:A:1512:U:H2'	3:A:1513:A:H8	1.77	0.48
3:A:1526:G:H8	3:A:1526:G:P	2.37	0.48
3:A:2877:G:N2	3:A:2880:A:OP2	2.42	0.48
1:N:7:ILE:HG23	22:D:13:THR:HG21	1.95	0.48
3:A:2361:U:OP2	10:M:17:ARG:NE	2.43	0.48
3:A:2784:A:H2'	3:A:2785:A:H5''	1.96	0.48
22:D:154:VAL:HG23	22:D:154:VAL:O	2.14	0.48
3:A:1423:C:O2'	3:A:1512:U:O2	2.19	0.48
3:A:303:G:H2'	3:A:304:G:H8	1.79	0.48
3:A:422:G:H2'	3:A:423:A:C8	2.48	0.48
3:A:1888:U:H2'	3:A:1889:G:C8	2.49	0.48
3:A:2792:A:H4'	3:A:2793:G:OP2	2.13	0.48
3:A:2171:G:N2	3:A:2173:U:O3'	2.47	0.48
3:A:1094:A:O2'	3:A:1095:A:O4'	2.31	0.48
3:A:1825:U:OP2	5:C:274:ARG:NH2	2.47	0.48
3:A:2819:C:H3'	3:A:2820:U:H6	1.79	0.48
12:P:36:ASP:OD1	12:P:36:ASP:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:45:GLN:NE2	14:S:57:LEU:HB2	2.29	0.48
3:A:2827:A:H2'	3:A:2828:U:O4'	2.14	0.48
9:K:54:MET:HB2	9:K:121:ALA:HB2	1.96	0.48
3:A:792:5MU:H4'	25:Q:92:ARG:HH22	1.79	0.47
3:A:2767:A:H2'	3:A:2768:A:C8	2.48	0.47
21:4:11:CYS:HB3	21:4:13:LYS:HG2	1.96	0.47
13:R:43:GLU:HG2	13:R:48:VAL:O	2.14	0.47
13:R:64:ARG:NE	13:R:69:GLN:HG2	2.29	0.47
16:U:19:LYS:O	16:U:22:ARG:NH1	2.47	0.47
18:3:58:VAL:HG23	18:3:58:VAL:O	2.14	0.47
3:A:1072:A:H2'	3:A:1073:A:C8	2.50	0.47
3:A:1823:U:H2'	3:A:1824:C:H6	1.77	0.47
3:A:2128:G:H2'	3:A:2129:C:C6	2.49	0.47
5:C:100:GLU:OE2	5:C:102:ARG:NH2	2.44	0.47
22:D:55:ASP:OD1	22:D:55:ASP:N	2.46	0.47
3:A:830:U:H2'	3:A:831:C:C6	2.49	0.47
3:A:1037:A:H62	3:A:1205:U:H3	1.62	0.47
3:A:1947:C:H2'	3:A:1948:G:C8	2.47	0.47
3:A:65:A:H2'	3:A:66:C:C6	2.49	0.47
3:A:293:U:C2	3:A:294:G:C8	3.01	0.47
3:A:1951:C:H2'	3:A:1952:C:C6	2.49	0.47
4:B:49:G:H2'	4:B:50:A:C8	2.50	0.47
15:T:46:VAL:O	15:T:50:LYS:HG2	2.15	0.47
22:D:169:MET:HE3	22:D:169:MET:HB3	1.74	0.47
3:A:287:G:H2'	3:A:288:C:O4'	2.14	0.47
3:A:939:U:P	3:A:940:U:H5	2.37	0.47
3:A:1395:G:H8	3:A:1410:A:H62	1.62	0.47
3:A:1570:G:H2'	3:A:1571:G:C8	2.50	0.47
3:A:2325:A:H3'	3:A:2326:G:H8	1.78	0.47
6:G:35:ARG:HE	6:G:71:LEU:HD13	1.80	0.47
14:S:43:LYS:O	14:S:56:ILE:HA	2.14	0.47
29:L:88:GLU:HA	29:L:91:GLU:HG3	1.95	0.47
3:A:290:U:C2	3:A:291:G:C8	3.03	0.47
3:A:1518:G:O2'	3:A:1519:U:H5'	2.14	0.47
3:A:2778:G:C5	6:G:3:ARG:HD3	2.49	0.47
25:Q:22:ASP:OD1	25:Q:25:ARG:NH2	2.48	0.47
3:A:787:U:H2'	3:A:788:A:C8	2.49	0.47
3:A:1241:A:H2'	3:A:1242:A:C8	2.50	0.47
3:A:1873:G:H2'	3:A:1874:A:C8	2.49	0.47
4:B:106:G:H2'	4:B:107:U:C6	2.49	0.47
10:M:72:LEU:HA	10:M:75:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1757:U:H2'	3:A:1758:A:O4'	2.15	0.47
3:A:1884:G:H21	3:A:1912:A:N6	2.08	0.47
3:A:2858:G:N2	3:A:2859:G:O6	2.48	0.47
11:O:98:ILE:HG12	12:P:2:PHE:HZ	1.79	0.47
3:A:460:C:H2'	3:A:461:A:C8	2.50	0.46
3:A:1450:A:H2'	3:A:1451:U:C6	2.49	0.46
3:A:1491:C:O2'	3:A:1492:G:H8	1.98	0.46
3:A:2347:A:HO2'	3:A:2349:A:N6	2.12	0.46
8:J:78:ASN:H	8:J:81:GLN:NE2	2.13	0.46
24:I:4:GLN:HG2	24:I:5:GLU:HG2	1.96	0.46
6:G:163:ARG:HG2	6:G:164:TYR:O	2.15	0.46
8:J:90:GLU:HA	8:J:122:THR:HG23	1.97	0.46
29:L:50:LEU:HD12	29:L:58:SER:HB2	1.98	0.46
3:A:1763:U:O2'	3:A:1767:G:O6	2.16	0.46
3:A:2155:C:H2'	3:A:2156:C:H6	1.79	0.46
3:A:2189:G:N2	3:A:2190:C:H41	2.13	0.46
3:A:2249:G:H2'	3:A:2250:A:O4'	2.15	0.46
24:I:115:VAL:HG13	24:I:121:VAL:HG21	1.98	0.46
3:A:460:C:H2'	3:A:461:A:H8	1.80	0.46
3:A:2676:U:H2'	3:A:2677:C:C6	2.51	0.46
3:A:1504:U:OP2	3:A:1504:U:H3'	2.16	0.46
4:B:42:G:N3	4:B:45:C:N4	2.55	0.46
1:N:90:ARG:HD3	1:N:114:GLU:OE2	2.14	0.46
3:A:1449:A:C8	3:A:1450:A:N6	2.83	0.46
3:A:943:C:H2'	3:A:944:G:H8	1.79	0.46
3:A:2784:A:N1	6:G:67:THR:HG21	2.31	0.46
3:A:275:A:N6	3:A:296:G:H21	2.07	0.46
4:B:106:G:H2'	4:B:107:U:H6	1.81	0.46
11:O:91:ASN:O	11:O:95:LEU:HB2	2.15	0.46
3:A:281:A:H2'	3:A:282:A:H8	1.79	0.46
3:A:878:C:H2'	3:A:879:U:C6	2.50	0.46
3:A:1238:U:H1'	11:O:4:VAL:HG22	1.98	0.46
3:A:1561:G:H8	3:A:1562:C:C6	2.34	0.46
3:A:1617:A:H2'	3:A:1618:A:C8	2.51	0.46
3:A:1902:G:N2	3:A:1903:A:H1'	2.28	0.46
3:A:2858:G:H5''	3:A:2859:G:OP1	2.15	0.46
4:B:31:G:H2'	4:B:32:U:C6	2.51	0.46
3:A:2177:U:H2'	3:A:2178:U:O4'	2.16	0.45
6:G:121:ILE:HD11	6:G:140:GLN:HG2	1.98	0.45
3:A:505:U:H2'	3:A:506:A:H5''	1.98	0.45
3:A:2495:A:HO2'	3:A:2496:A:P	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1457:U:O4	3:A:1458:A:N6	2.49	0.45
3:A:1491:C:O2'	3:A:1492:G:O5'	2.30	0.45
25:Q:28:ASN:HA	25:Q:70:VAL:HA	1.98	0.45
2:E:146:LEU:O	2:E:146:LEU:HD12	2.17	0.45
3:A:925:G:H2'	3:A:926:G:O4'	2.17	0.45
3:A:331:G:H1	3:A:395:U:H3	1.64	0.45
3:A:756:A:H2'	3:A:757:G:O4'	2.16	0.45
3:A:1395:G:C2	3:A:1408:G:N7	2.85	0.45
24:I:35:ILE:HD11	24:I:65:THR:H	1.82	0.45
3:A:289:U:H2'	3:A:290:U:H6	1.81	0.45
3:A:304:G:N7	3:A:410:G:N2	2.46	0.45
3:A:926:G:O6	3:A:938:G:H5''	2.16	0.45
3:A:1475:A:N6	3:A:1606:C:O2	2.50	0.45
3:A:2147:G:N3	3:A:2206:C:N4	2.60	0.45
3:A:1875:A:HO2'	3:A:1876:G:H8	1.63	0.45
3:A:2346:U:H5'	3:A:2348:G:O6	2.16	0.45
19:1:9:CYS:HB3	19:1:12:CYS:HB2	1.87	0.45
3:A:942:C:H2'	3:A:943:C:C6	2.52	0.45
3:A:1631:G:O3'	3:A:1632:A:H8	2.00	0.45
3:A:2858:G:O2'	3:A:2859:G:C8	2.62	0.45
29:L:96:ARG:HA	29:L:96:ARG:HD2	1.80	0.45
3:A:805:G:H2'	3:A:806:A:O4'	2.17	0.45
4:B:27:A:H2'	4:B:28:C:H6	1.80	0.45
4:B:58:C:C2	4:B:59:U:C5	3.05	0.45
2:E:49:HIS:ND1	2:E:92:PRO:HB2	2.32	0.45
2:E:146:LEU:O	2:E:148:GLN:HG2	2.17	0.45
3:A:2321:C:OP1	10:M:96:ARG:NH1	2.42	0.45
3:A:2354:A:H2'	3:A:2355:A:C8	2.52	0.45
4:B:49:G:C6	4:B:50:A:C6	3.04	0.45
11:O:105:ALA:HB1	12:P:40:PHE:HZ	1.80	0.45
3:A:2581:U:H2'	3:A:2582:U:C6	2.52	0.44
4:B:71:A:N7	4:B:100:U:H5	2.15	0.44
6:G:67:THR:O	6:G:71:LEU:HG	2.17	0.44
7:H:76:TYR:HA	7:H:86:LYS:O	2.17	0.44
15:T:44:ASP:OD2	15:T:47:GLU:HG3	2.17	0.44
17:W:48:LYS:HD3	17:W:48:LYS:HA	1.70	0.44
27:X:12:VAL:CG2	27:X:20:ARG:HG2	2.47	0.44
29:L:18:ARG:HG2	29:L:65:THR:HG23	1.97	0.44
3:A:1455:U:H1'	3:A:1457:U:C4	2.53	0.44
3:A:2259:C:OP2	26:V:27:ARG:NH2	2.49	0.44
4:B:84:U:HO2'	4:B:86:A:H2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:43:VAL:HG23	7:H:44:THR:HG23	1.98	0.44
3:A:637:U:H2'	3:A:638:U:C6	2.52	0.44
3:A:1455:U:H1'	3:A:1457:U:O4	2.17	0.44
3:A:1945:A:N3	3:A:1945:A:H2'	2.33	0.44
2:E:13:LYS:HG2	2:E:14:SER:O	2.17	0.44
3:A:282:A:H2'	3:A:283:G:C8	2.52	0.44
3:A:294:G:H2'	3:A:295:G:C8	2.52	0.44
3:A:2326:G:H2'	3:A:2327:A:C8	2.52	0.44
3:A:2331:G:N2	3:A:2334:G:H22	2.16	0.44
3:A:2580:G:C2	3:A:2610:G:H1'	2.52	0.44
5:C:69:ARG:O	5:C:189:ARG:NH1	2.50	0.44
3:A:215:G:H2'	3:A:216:A:O4'	2.18	0.44
3:A:307:A:H2'	3:A:308:C:C6	2.52	0.44
3:A:942:C:H2'	3:A:943:C:H6	1.83	0.44
3:A:1582:U:O2'	3:A:1585:G:O6	2.36	0.44
3:A:2774:G:O2'	6:G:67:THR:HG22	2.17	0.44
4:B:73:G:O2'	15:T:88:HIS:HE1	2.00	0.44
9:K:43:THR:O	9:K:44:SER:HB3	2.16	0.44
3:A:901:G:H2'	3:A:902:A:C8	2.53	0.44
18:3:59:LYS:HB3	18:3:59:LYS:HE2	1.75	0.44
3:A:1057:A:O2'	3:A:1058:U:H6	2.00	0.44
3:A:1501:G:H2'	3:A:1502:A:C8	2.53	0.44
3:A:1758:A:H1'	3:A:1772:G:N1	2.33	0.44
3:A:2183:G:H2'	3:A:2184:G:O4'	2.18	0.44
3:A:2820:U:O2'	3:A:2823:G:O6	2.30	0.44
4:B:27:A:OP2	10:M:36:SER:OG	2.36	0.44
6:G:119:GLU:O	6:G:121:ILE:HG12	2.17	0.44
8:J:23:VAL:CG2	12:P:81:ASN:HB3	2.48	0.44
3:A:409:G:H2'	3:A:410:G:H5'	1.99	0.43
3:A:766:G:H2'	3:A:767:A:C8	2.53	0.43
3:A:809:A:H61	3:A:1816:A:H8	1.66	0.43
3:A:1526:G:H1'	3:A:1553:A:N1	2.33	0.43
3:A:2334:G:O2'	3:A:2337:A:OP2	2.26	0.43
2:E:66:LYS:HB2	2:E:66:LYS:HE3	1.69	0.43
3:A:877:G:H2'	3:A:878:C:C6	2.53	0.43
4:B:40:C:H2'	4:B:41:C:C6	2.53	0.43
15:T:12:LYS:HD2	15:T:12:LYS:HA	1.70	0.43
3:A:436:A:H1'	3:A:437:A:C8	2.54	0.43
3:A:579:U:O2'	11:O:49:ASP:OD2	2.23	0.43
3:A:1758:A:N1	3:A:1766:C:O2'	2.41	0.43
4:B:45:C:C2	4:B:46:A:C8	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:48:A:OP1	10:M:70:VAL:HG23	2.18	0.43
6:G:144:LEU:O	6:G:148:ILE:HG23	2.18	0.43
27:X:6:ILE:HD12	27:X:56:VAL:HG22	2.01	0.43
3:A:310:C:C4	3:A:311:U:C4	3.06	0.43
3:A:684:U:H2'	3:A:685:C:H6	1.81	0.43
3:A:1089:C:OP1	3:A:1091:G:O2'	2.35	0.43
3:A:1680:U:H2'	3:A:1681:U:C6	2.54	0.43
3:A:1816:A:H2'	3:A:1817:C:O4'	2.19	0.43
4:B:37:A:H2'	4:B:38:U:C6	2.54	0.43
6:G:12:PRO:HD3	6:G:49:THR:HA	2.00	0.43
6:G:26:VAL:O	6:G:32:GLU:N	2.51	0.43
23:F:93:GLY:O	23:F:97:TYR:N	2.43	0.43
3:A:273:A:OP2	3:A:297:G:N1	2.41	0.43
3:A:766:G:H2'	3:A:767:A:H8	1.84	0.43
24:I:7:ARG:HB3	24:I:18:GLU:OE2	2.18	0.43
3:A:774:G:H1'	3:A:809:A:OP1	2.19	0.43
3:A:1013:U:H2'	3:A:1014:U:C6	2.54	0.43
3:A:1496:G:N7	3:A:1502:A:N1	2.67	0.43
3:A:1588:U:H2'	3:A:1589:U:O4'	2.19	0.43
3:A:1625:U:H2'	3:A:1626:A:C8	2.53	0.43
3:A:2343:U:H2'	3:A:2344:C:H6	1.82	0.43
4:B:46:A:H2'	4:B:47:C:C6	2.54	0.43
7:H:60:ALA:HB3	7:H:126:TYR:O	2.19	0.43
11:O:88:ILE:HG22	11:O:90:ILE:HG13	2.00	0.43
3:A:65:A:H2'	3:A:66:C:H6	1.84	0.43
3:A:287:G:O5'	3:A:287:G:H8	2.01	0.43
3:A:1091:G:O2'	3:A:1155:A:N6	2.51	0.43
11:O:58:ARG:HA	11:O:61:TRP:CE3	2.53	0.43
11:O:88:ILE:H	11:O:88:ILE:HG12	1.55	0.43
3:A:620:G:O2'	3:A:1292:A:OP1	2.37	0.43
3:A:297:G:H2'	3:A:298:U:C6	2.53	0.43
2:E:21:ASP:HA	2:E:24:PHE:O	2.18	0.43
3:A:1882:G:H2'	3:A:1883:A:H8	1.84	0.43
3:A:2048:G:H2'	3:A:2048:G:N3	2.34	0.43
3:A:2142:G:H2'	3:A:2143:G:H8	1.84	0.43
3:A:2332:U:C2	23:F:151:GLY:HA3	2.54	0.43
25:Q:2:GLU:HG2	25:Q:108:SER:HB3	2.01	0.43
3:A:1477:U:H2'	3:A:1478:A:C8	2.54	0.42
3:A:1911:A:C2	3:A:1912:A:C8	3.07	0.42
4:B:37:A:H2	4:B:42:G:C4	2.37	0.42
22:D:55:ASP:HA	22:D:84:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:42:VAL:HG12	29:L:105:LYS:O	2.19	0.42
3:A:1017:A:H5''	12:P:80:LYS:HD2	2.01	0.42
3:A:1525:U:C2	3:A:1551:U:H5'	2.54	0.42
3:A:1637:A:H2'	3:A:1638:G:O4'	2.18	0.42
3:A:2153:A:N7	3:A:2191:U:O2'	2.43	0.42
3:A:2448:G:H2'	3:A:2449:C:C6	2.54	0.42
4:B:2:C:H2'	4:B:3:U:C6	2.55	0.42
15:T:25:GLY:O	15:T:45:GLU:N	2.47	0.42
2:E:10:ASP:OD1	2:E:10:ASP:N	2.49	0.42
3:A:745:G:O2'	3:A:1676:A:N3	2.46	0.42
3:A:1089:C:N4	3:A:1155:A:O2'	2.51	0.42
3:A:2819:C:H3'	3:A:2820:U:C6	2.54	0.42
21:4:30:PRO:O	21:4:33:LYS:HG2	2.19	0.42
3:A:422:G:H2'	3:A:423:A:H8	1.84	0.42
3:A:808:G:H3'	3:A:808:G:C8	2.54	0.42
3:A:1577:G:H2'	3:A:1578:A:C2	2.55	0.42
4:B:2:C:N3	4:B:114:G:N2	2.68	0.42
8:J:23:VAL:HG21	12:P:81:ASN:HB3	2.02	0.42
24:I:98:ILE:HD12	24:I:117:LEU:HB2	2.01	0.42
3:A:525:A:N3	3:A:527:G:H5''	2.34	0.42
3:A:1562:C:H2'	3:A:1563:U:C6	2.54	0.42
3:A:2825:U:H2'	3:A:2826:U:O4'	2.19	0.42
4:B:59:U:H2'	4:B:60:C:H6	1.84	0.42
6:G:152:ARG:HA	6:G:152:ARG:HD3	1.83	0.42
5:C:168:GLU:N	5:C:168:GLU:OE1	2.52	0.42
10:M:19:ARG:HE	10:M:30:ARG:CZ	2.32	0.42
2:E:183:VAL:O	2:E:187:THR:HG23	2.20	0.42
3:A:291:G:H2'	3:A:292:U:C6	2.55	0.42
3:A:1876:G:H2'	3:A:1877:G:O4'	2.20	0.42
5:C:4:LYS:HG2	5:C:18:SER:O	2.20	0.42
3:A:292:U:H2'	3:A:293:U:H6	1.83	0.42
3:A:946:A:H2'	3:A:947:U:C6	2.55	0.42
3:A:1194:U:O2'	3:A:1195:A:H5''	2.20	0.42
3:A:1550:G:H5'	3:A:1552:U:H5	1.85	0.42
3:A:2318:U:H2'	3:A:2319:U:H6	1.83	0.42
7:H:3:GLN:HE22	12:P:13:LYS:H	1.68	0.42
3:A:1487:G:H1	3:A:1596:G:N2	2.16	0.42
3:A:2626:G:OP2	5:C:235:GLY:HA2	2.20	0.42
3:A:2916:U:H2'	3:A:2917:U:C6	2.54	0.42
22:D:99:TYR:HA	22:D:103:GLN:OE1	2.20	0.42
26:V:40:VAL:HG12	26:V:41:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3:U:H2'	3:A:4:U:C6	2.55	0.41
3:A:304:G:C4	3:A:305:A:C8	3.08	0.41
3:A:2342:U:H2'	3:A:2343:U:C6	2.55	0.41
4:B:47:C:H2'	4:B:48:A:H8	1.84	0.41
3:A:650:U:C5	3:A:665:G:C5	3.08	0.41
18:3:22:LEU:HD12	18:3:55:MET:SD	2.60	0.41
3:A:576:U:H5	3:A:2045:A:N1	2.19	0.41
3:A:940:U:C2	3:A:941:A:C8	3.07	0.41
3:A:2650:G:O5'	3:A:2845:G:N2	2.52	0.41
3:A:872:U:O2'	3:A:2095:U:C2	2.64	0.41
3:A:1301:U:C4	3:A:1302:G:C6	3.08	0.41
3:A:1457:U:H2'	3:A:1458:A:O4'	2.20	0.41
3:A:1909:C:H2'	3:A:1910:G:O4'	2.20	0.41
3:A:326:A:HO2'	3:A:327:G:H8	1.68	0.41
3:A:1151:G:H2'	3:A:1152:U:H6	1.84	0.41
3:A:1465:G:C2	3:A:1466:G:C8	3.08	0.41
3:A:1504:U:O2'	3:A:1505:G:OP2	2.37	0.41
3:A:1579:C:H2'	3:A:1581:U:O2	2.20	0.41
3:A:2107:G:H5'	26:V:19:SER:HB2	2.02	0.41
3:A:2158:U:H5''	3:A:2160:G:N7	2.35	0.41
4:B:64:A:N6	4:B:104:A:H2'	2.35	0.41
13:R:14:GLU:H	13:R:14:GLU:HG2	1.65	0.41
24:I:65:THR:O	24:I:79:PHE:HB2	2.21	0.41
3:A:1490:G:O5'	3:A:1490:G:C8	2.73	0.41
3:A:1526:G:H2'	3:A:1527:A:C8	2.55	0.41
3:A:1904:A:C5	3:A:1905:G:C8	3.09	0.41
3:A:2300:A:H2'	3:A:2301:A:C8	2.55	0.41
3:A:2803:A:H4'	3:A:2804:G:H5''	2.03	0.41
4:B:47:C:H2'	4:B:48:A:C8	2.56	0.41
10:M:89:ILE:C	10:M:90:LYS:HD2	2.40	0.41
3:A:1555:G:H2'	3:A:1557:C:H5	1.84	0.41
4:B:27:A:P	10:M:36:SER:HG	2.44	0.41
4:B:46:A:H2'	4:B:47:C:H6	1.85	0.41
3:A:969:A:HO2'	3:A:970:U:H6	1.65	0.41
3:A:1515:G:N2	3:A:1565:U:H3	1.98	0.41
3:A:2200:A:H3'	3:A:2201:C:C6	2.56	0.41
3:A:2499:G:N2	3:A:2505:A:H62	2.19	0.41
6:G:8:ILE:HA	6:G:69:ARG:HE	1.86	0.41
7:H:12:ILE:HD13	7:H:50:ASP:O	2.21	0.41
7:H:24:GLN:HE21	7:H:24:GLN:HB3	1.73	0.41
15:T:4:LEU:HD12	15:T:4:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1090:A:H5''	3:A:1091:G:C8	2.56	0.41
3:A:1212:U:H2'	3:A:1213:C:C6	2.56	0.41
3:A:1821:U:H2'	3:A:1822:C:C6	2.56	0.41
3:A:1912:A:H2'	3:A:1913:U:O4'	2.21	0.41
3:A:2334:G:H3'	3:A:2335:G:H4'	2.03	0.41
3:A:2335:G:H2'	3:A:2337:A:H62	1.86	0.41
3:A:2705:U:O2'	3:A:2706:A:C8	2.73	0.41
8:J:55:LEU:HD23	8:J:60:ARG:HB3	2.03	0.41
10:M:38:LYS:HA	10:M:38:LYS:HD2	1.94	0.41
13:R:62:LYS:HG2	13:R:71:TYR:CE2	2.56	0.41
17:W:2:LYS:HB3	17:W:2:LYS:HE3	1.78	0.41
22:D:108:ASP:OD1	22:D:108:ASP:N	2.48	0.41
24:I:111:PHE:O	24:I:115:VAL:HG23	2.21	0.41
27:X:23:VAL:HG23	27:X:50:VAL:HG21	2.03	0.41
3:A:1569:G:H5''	3:A:1570:G:C8	2.56	0.41
3:A:1573:A:N6	3:A:1592:A:H62	2.18	0.41
3:A:1627:G:H2'	3:A:1628:A:H8	1.85	0.41
3:A:1876:G:H2'	3:A:1877:G:C8	2.55	0.41
3:A:2202:U:H2'	3:A:2203:A:H8	1.85	0.41
6:G:27:LYS:HE2	6:G:27:LYS:HB2	1.95	0.41
8:J:20:GLY:HA2	8:J:28:GLY:O	2.21	0.41
3:A:303:G:H2'	3:A:304:G:C8	2.56	0.40
3:A:1082:C:H42	3:A:1161:A:H61	1.69	0.40
3:A:1357:G:C2	3:A:1366:U:H5''	2.55	0.40
3:A:1950:U:H2'	3:A:1951:C:C6	2.56	0.40
3:A:2144:A:H2'	3:A:2176:C:H5'	2.03	0.40
7:H:19:ILE:HD13	7:H:141:TYR:HB3	2.03	0.40
15:T:49:ILE:HA	15:T:52:ILE:HG22	2.03	0.40
3:A:291:G:H2'	3:A:292:U:H6	1.87	0.40
3:A:922:G:C2	3:A:923:A:C5	3.08	0.40
6:G:104:ILE:HA	6:G:113:VAL:O	2.21	0.40
7:H:15:LYS:O	7:H:53:ASP:HB3	2.21	0.40
8:J:93:PRO:HD3	8:J:124:LYS:O	2.21	0.40
9:K:44:SER:HB2	9:K:70:PRO:HG3	2.02	0.40
1:N:99:LEU:HB3	1:N:102:LEU:HD23	2.02	0.40
3:A:78:U:H2'	3:A:79:U:C6	2.56	0.40
3:A:992:A:H1'	3:A:1028:G:C8	2.56	0.40
3:A:1216:U:C2'	3:A:1217:U:H5'	2.51	0.40
3:A:1453:G:C4'	3:A:1631:G:H22	2.33	0.40
3:A:1478:A:H61	3:A:1605:A:H61	1.69	0.40
3:A:1759:G:N7	3:A:1761:G:N2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2078:A:H4'	22:D:154:VAL:HG22	2.03	0.40
3:A:2212:G:H2'	3:A:2213:U:C6	2.56	0.40
4:B:1:U:H3	4:B:114:G:H1	1.69	0.40
7:H:103:GLU:HG2	7:H:107:LYS:HE2	2.02	0.40
10:M:32:ASN:OD1	10:M:33:VAL:N	2.54	0.40
14:S:95:LYS:HA	14:S:95:LYS:HD2	1.91	0.40
3:A:410:G:O2'	3:A:411:A:N7	2.45	0.40
3:A:1350:U:H5	3:A:1647:A:N1	2.19	0.40
3:A:1452:C:H2'	3:A:1453:G:C2	2.56	0.40
3:A:2331:G:N2	3:A:2339:U:H3	2.17	0.40
9:K:67:LYS:HB3	9:K:67:LYS:HE2	1.78	0.40
10:M:79:ALA:O	10:M:82:LYS:HG2	2.22	0.40
14:S:57:LEU:HD12	14:S:58:GLU:H	1.87	0.40
26:V:35:LYS:HE3	26:V:46:LYS:HG2	2.04	0.40
3:A:324:A:H2'	3:A:325:A:O4'	2.22	0.40
3:A:1039:C:C5	7:H:2:ARG:HG2	2.56	0.40
3:A:1585:G:H5'	3:A:1586:U:C5	2.56	0.40
3:A:1882:G:H2'	3:A:1883:A:C8	2.57	0.40
3:A:1913:U:H2'	3:A:1914:C:C6	2.56	0.40
3:A:2128:G:O6	3:A:2215:U:O4	2.40	0.40
3:A:2146:A:H1'	3:A:2199:U:C2	2.57	0.40
3:A:2707:C:OP1	22:D:123:LYS:HG2	2.21	0.40
5:C:227:PRO:HA	5:C:233:GLY:HA3	2.04	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
1	N	112/114 (98%)	106 (95%)	6 (5%)	0	100 100
2	E	204/206 (99%)	197 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	272/274 (99%)	259 (95%)	13 (5%)	0	100	100
6	G	173/175 (99%)	155 (90%)	18 (10%)	0	100	100
7	H	143/145 (99%)	124 (87%)	18 (13%)	1 (1%)	22	36
8	J	144/146 (99%)	135 (94%)	8 (6%)	1 (1%)	22	36
9	K	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
10	M	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	17	29
11	O	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
12	P	100/102 (98%)	92 (92%)	7 (7%)	1 (1%)	15	26
13	R	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
14	S	96/104 (92%)	81 (84%)	15 (16%)	0	100	100
15	T	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
16	U	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
17	W	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
18	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
19	1	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
20	2	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
21	4	35/37 (95%)	35 (100%)	0	0	100	100
22	D	213/215 (99%)	179 (84%)	27 (13%)	7 (3%)	4	4
23	F	156/158 (99%)	141 (90%)	15 (10%)	0	100	100
24	I	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
25	Q	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
26	V	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
27	X	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
28	Z	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
29	L	118/120 (98%)	106 (90%)	11 (9%)	1 (1%)	19	33
All	All	2980/3040 (98%)	2750 (92%)	218 (7%)	12 (0%)	38	52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	D	130	ALA
29	L	67	ARG
22	D	158	SER

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Mol	Chain	Res	Type
22	D	164	PHE
8	J	36	LYS
22	D	143	HIS
7	H	77	ARG
10	M	68	THR
22	D	172	ARG
12	P	51	PRO
22	D	171	GLY
22	D	124	GLY

### 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	
1	N	93/100 (93%)	93 (100%)	0	100	100
2	E	168/168 (100%)	167 (99%)	1 (1%)	86	94
5	C	221/221 (100%)	221 (100%)	0	100	100
6	G	124/153 (81%)	122 (98%)	2 (2%)	62	82
7	H	123/123 (100%)	123 (100%)	0	100	100
8	J	109/112 (97%)	109 (100%)	0	100	100
9	K	108/114 (95%)	108 (100%)	0	100	100
10	M	83/95 (87%)	82 (99%)	1 (1%)	71	87
11	O	96/96 (100%)	95 (99%)	1 (1%)	76	89
12	P	84/86 (98%)	82 (98%)	2 (2%)	49	72
13	R	78/80 (98%)	78 (100%)	0	100	100
14	S	81/89 (91%)	81 (100%)	0	100	100
15	T	78/82 (95%)	78 (100%)	0	100	100
16	U	59/62 (95%)	59 (100%)	0	100	100
17	W	58/60 (97%)	58 (100%)	0	100	100
18	3	55/55 (100%)	55 (100%)	0	100	100
19	1	44/45 (98%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	2	39/39 (100%)	39 (100%)	0	100	100
21	4	35/35 (100%)	35 (100%)	0	100	100
22	D	173/173 (100%)	167 (96%)	6 (4%)	36	59
24	I	100/100 (100%)	99 (99%)	1 (1%)	76	89
25	Q	89/91 (98%)	89 (100%)	0	100	100
26	V	39/41 (95%)	38 (97%)	1 (3%)	46	70
27	X	52/52 (100%)	52 (100%)	0	100	100
28	Z	35/44 (80%)	35 (100%)	0	100	100
29	L	94/101 (93%)	93 (99%)	1 (1%)	73	88
All	All	2318/2417 (96%)	2302 (99%)	16 (1%)	84	93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	41	ARG
6	G	44	LYS
6	G	175	LYS
10	M	59	LYS
11	O	88	ILE
12	P	1	MET
12	P	52	THR
22	D	25	VAL
22	D	107	VAL
22	D	125	LYS
22	D	133	ARG
22	D	159	ASP
22	D	173	MET
24	I	122	LEU
26	V	27	ARG
29	L	122	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	4	HIS
2	E	162	ASN
5	C	90	ASN
6	G	106	ASN

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Mol	Chain	Res	Type
7	H	24	GLN
7	H	59	ASN
7	H	81	HIS
8	J	54	GLN
8	J	70	ASN
8	J	81	GLN
9	K	25	ASN
10	M	15	HIS
10	M	43	GLN
10	M	102	HIS
12	P	18	GLN
12	P	65	GLN
14	S	44	HIS
14	S	45	GLN
15	T	88	HIS
16	U	20	ASN
18	3	60	GLN
19	1	16	ASN
20	2	7	GLN
22	D	33	ASN
22	D	37	GLN
22	D	47	ASN
22	D	50	GLN
22	D	143	HIS
24	I	110	ASN
25	Q	60	HIS
26	V	16	ASN
28	Z	19	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	A	2823/2923 (96%)	445 (15%)	12 (0%)
4	B	114/115 (99%)	13 (11%)	0
All	All	2937/3038 (96%)	458 (15%)	12 (0%)

All (458) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A	10	A
3	A	28	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	34	U
3	A	36	G
3	A	43	A
3	A	58	G
3	A	63	U
3	A	64	A
3	A	71	A
3	A	75	G
3	A	90	A
3	A	109	G
3	A	118	A
3	A	119	U
3	A	140	A
3	A	164	A
3	A	177	G
3	A	184	C
3	A	185	A
3	A	199	A
3	A	202	A
3	A	216	A
3	A	218	G
3	A	219	A
3	A	225	A
3	A	231	A
3	A	233	U
3	A	236	A
3	A	242	U
3	A	248	G
3	A	251	G
3	A	255	G
3	A	272	C
3	A	279	A
3	A	285	U
3	A	286	U
3	A	298	U
3	A	302	A
3	A	306	C
3	A	307	A
3	A	310	C
3	A	316	G
3	A	321	U
3	A	324	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	326	A
3	A	327	G
3	A	328	G
3	A	335	U
3	A	373	A
3	A	389	A
3	A	397	U
3	A	404	U
3	A	432	G
3	A	433	U
3	A	457	G
3	A	463	C
3	A	466	C
3	A	481	C
3	A	486	G
3	A	490	C
3	A	503	A
3	A	505	U
3	A	506	A
3	A	513	G
3	A	518	A
3	A	527	G
3	A	538	G
3	A	550	A
3	A	553	A
3	A	554	C
3	A	567	G
3	A	575	G
3	A	576	U
3	A	577	A
3	A	583	A
3	A	587	C
3	A	591	A
3	A	592	A
3	A	594	G
3	A	606	G
3	A	616	G
3	A	618	A
3	A	630	G
3	A	646	A
3	A	659	A
3	A	660	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	666	A
3	A	679	G
3	A	682	A
3	A	690	U
3	A	698	U
3	A	699	U
3	A	713	A
3	A	720	A
3	A	731	U
3	A	745	G
3	A	751	A
3	A	766	G
3	A	775	A
3	A	783	G
3	A	792	5MU
3	A	793	G
3	A	797	A
3	A	809	A
3	A	810	A
3	A	820	G
3	A	823	G
3	A	827	A
3	A	829	U
3	A	834	A
3	A	835	U
3	A	837	G
3	A	850	G
3	A	857	C
3	A	868	A
3	A	872	U
3	A	891	A
3	A	904	G
3	A	908	A
3	A	911	A
3	A	922	G
3	A	940	U
3	A	955	A
3	A	968	A
3	A	970	U
3	A	971	U
3	A	977	A
3	A	989	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	990	G
3	A	1005	G
3	A	1018	A
3	A	1019	A
3	A	1027	A
3	A	1037	A
3	A	1040	A
3	A	1053	A
3	A	1056	U
3	A	1057	A
3	A	1058	U
3	A	1059	A
3	A	1060	U
3	A	1061	G
3	A	1070	A
3	A	1077	U
3	A	1079	U
3	A	1083	G
3	A	1088	C
3	A	1089	C
3	A	1090	A
3	A	1091	G
3	A	1094	A
3	A	1095	A
3	A	1154	G
3	A	1155	A
3	A	1156	G
3	A	1163	U
3	A	1166	G
3	A	1172	A
3	A	1174	U
3	A	1176	U
3	A	1178	C
3	A	1179	C
3	A	1186	A
3	A	1187	A
3	A	1190	A
3	A	1191	U
3	A	1192	A
3	A	1193	U
3	A	1194	U
3	A	1196	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	1216	U
3	A	1217	U
3	A	1220	A
3	A	1258	A
3	A	1288	G
3	A	1291	A
3	A	1294	G
3	A	1300	G
3	A	1309	G
3	A	1310	A
3	A	1312	A
3	A	1320	G
3	A	1321	A
3	A	1326	C
3	A	1337	A
3	A	1338	U
3	A	1339	U
3	A	1344	A
3	A	1350	U
3	A	1358	A
3	A	1378	U
3	A	1382	C
3	A	1389	U
3	A	1397	G
3	A	1402	A
3	A	1405	G
3	A	1407	C
3	A	1416	U
3	A	1421	A
3	A	1449	A
3	A	1450	A
3	A	1451	U
3	A	1453	G
3	A	1454	U
3	A	1455	U
3	A	1459	A
3	A	1463	A
3	A	1464	U
3	A	1465	G
3	A	1472	C
3	A	1473	G
3	A	1490	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	1491	C
3	A	1492	G
3	A	1495	C
3	A	1496	G
3	A	1503	U
3	A	1504	U
3	A	1505	G
3	A	1507	A
3	A	1519	U
3	A	1520	A
3	A	1521	A
3	A	1525	U
3	A	1532	U
3	A	1552	U
3	A	1553	A
3	A	1555	G
3	A	1559	G
3	A	1561	G
3	A	1570	G
3	A	1578	A
3	A	1579	C
3	A	1581	U
3	A	1582	U
3	A	1583	G
3	A	1584	U
3	A	1586	U
3	A	1592	A
3	A	1594	U
3	A	1605	A
3	A	1606	C
3	A	1613	G
3	A	1616	A
3	A	1630	A
3	A	1631	G
3	A	1632	A
3	A	1639	G
3	A	1651	C
3	A	1653	A
3	A	1676	A
3	A	1690	A
3	A	1691	G
3	A	1692	C

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	1698	A
3	A	1718	G
3	A	1731	G
3	A	1740	G
3	A	1757	U
3	A	1761	G
3	A	1765	A
3	A	1768	C
3	A	1770	C
3	A	1771	A
3	A	1772	G
3	A	1790	G
3	A	1791	G
3	A	1797	G
3	A	1800	A
3	A	1803	G
3	A	1809	C
3	A	1826	G
3	A	1827	C
3	A	1828	U
3	A	1843	U
3	A	1856	A
3	A	1860	C
3	A	1893	A
3	A	1894	G
3	A	1898	C
3	A	1903	A
3	A	1904	A
3	A	1909	C
3	A	1918	G
3	A	1933	G
3	A	1938	U
3	A	1945	A
3	A	1946	A
3	A	1956	G
3	A	1957	G
3	A	1963	A
3	A	1965	A
3	A	1982	U
3	A	1992	C
3	A	1994	C
3	A	1996	A

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	1997	A
3	A	1998	A
3	A	1999	G
3	A	2003	U
3	A	2014	G
3	A	2018	U
3	A	2020	U
3	A	2050	A
3	A	2054	G
3	A	2058	A
3	A	2059	G
3	A	2060	A
3	A	2065	G
3	A	2070	C
3	A	2078	A
3	A	2082	C
3	A	2083	G
3	A	2087	A
3	A	2088	G
3	A	2089	A
3	A	2096	G
3	A	2107	G
3	A	2120	G
3	A	2138	U
3	A	2139	A
3	A	2143	G
3	A	2145	U
3	A	2146	A
3	A	2147	G
3	A	2153	A
3	A	2158	U
3	A	2160	G
3	A	2165	G
3	A	2172	C
3	A	2173	U
3	A	2185	A
3	A	2186	G
3	A	2190	C
3	A	2193	G
3	A	2194	U
3	A	2195	G
3	A	2196	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	2198	A
3	A	2210	C
3	A	2225	A
3	A	2230	G
3	A	2231	C
3	A	2238	U
3	A	2239	A
3	A	2247	G
3	A	2252	A
3	A	2265	G
3	A	2266	G
3	A	2295	A
3	A	2306	G
3	A	2310	C
3	A	2314	A
3	A	2321	C
3	A	2332	U
3	A	2334	G
3	A	2335	G
3	A	2346	U
3	A	2347	A
3	A	2352	G
3	A	2362	A
3	A	2374	C
3	A	2377	C
3	A	2378	G
3	A	2388	A
3	A	2396	A
3	A	2410	G
3	A	2412	C
3	A	2417	U
3	A	2427	G
3	A	2429	U
3	A	2433	C
3	A	2456	G
3	A	2457	A
3	A	2460	A
3	A	2461	A
3	A	2462	A
3	A	2468	C
3	A	2474	G
3	A	2475	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	2496	A
3	A	2500	U
3	A	2503	A
3	A	2505	A
3	A	2528	C
3	A	2529	G
3	A	2531	U
3	A	2545	A
3	A	2547	C
3	A	2556	G
3	A	2557	U
3	A	2579	U
3	A	2589	U
3	A	2593	A
3	A	2594	G
3	A	2599	A
3	A	2600	C
3	A	2613	C
3	A	2629	A
3	A	2630	G
3	A	2635	G
3	A	2636	U
3	A	2640	U
3	A	2642	U
3	A	2648	G
3	A	2657	G
3	A	2679	U
3	A	2681	A
3	A	2692	A
3	A	2699	U
3	A	2700	G
3	A	2706	A
3	A	2712	G
3	A	2716	U
3	A	2741	G
3	A	2753	U
3	A	2771	G
3	A	2775	A
3	A	2778	G
3	A	2785	A
3	A	2792	A
3	A	2796	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	2804	G
3	A	2805	A
3	A	2806	U
3	A	2807	G
3	A	2817	A
3	A	2818	A
3	A	2823	G
3	A	2826	U
3	A	2828	U
3	A	2841	A
3	A	2842	G
3	A	2845	G
3	A	2855	A
3	A	2858	G
3	A	2859	G
3	A	2887	G
3	A	2892	G
3	A	2900	C
3	A	2901	U
3	A	2903	A
3	A	2904	U
3	A	2913	G
3	A	2915	C
4	B	10	U
4	B	11	A
4	B	23	U
4	B	24	C
4	B	33	U
4	B	39	G
4	B	40	C
4	B	55	A
4	B	61	C
4	B	87	C
4	B	88	G
4	B	106	G
4	B	115	C

All (12) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	576	U
3	A	793	G

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Mol	Chain	Res	Type
3	A	808	G
3	A	872	U
3	A	1452	C
3	A	2064	A
3	A	2495	A
3	A	2528	C
3	A	2629	A
3	A	2840	A
3	A	2858	G
3	A	2900	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	2MA	A	2530	3	17,25,26	2.22	5 (29%)	17,37,40	1.47	3 (17%)
3	5MU	A	792	3	19,22,23	4.74	7 (36%)	28,32,35	3.81	11 (39%)
3	5MU	A	1966	3	19,22,23	4.75	7 (36%)	28,32,35	3.72	9 (32%)

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
3	2MA	A	2530	3	-	2/3/25/26	0/3/3/3
3	5MU	A	792	3	-	2/7/25/26	0/2/2/2
3	5MU	A	1966	3	-	0/7/25/26	0/2/2/2

All (19) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	792	5MU	C2-N1	10.82	1.55	1.38
3	A	1966	5MU	C2-N1	10.55	1.55	1.38
3	A	1966	5MU	C6-N1	10.27	1.55	1.38
3	A	792	5MU	C6-N1	10.06	1.55	1.38
3	A	1966	5MU	C4-C5	9.58	1.60	1.44
3	A	792	5MU	C4-C5	9.07	1.59	1.44
3	A	792	5MU	C4-N3	-8.16	1.23	1.38
3	A	1966	5MU	C4-N3	-7.79	1.24	1.38
3	A	1966	5MU	C6-C5	6.11	1.44	1.34
3	A	2530	2MA	C2-N3	6.04	1.44	1.31
3	A	792	5MU	C6-C5	5.89	1.44	1.34
3	A	2530	2MA	C4-N3	4.29	1.47	1.37
3	A	792	5MU	O4-C4	-3.58	1.16	1.23
3	A	2530	2MA	C5-C4	-3.46	1.34	1.43
3	A	1966	5MU	O4-C4	-3.26	1.17	1.23
3	A	792	5MU	O2-C2	-3.05	1.17	1.23
3	A	1966	5MU	O2-C2	-2.98	1.17	1.23
3	A	2530	2MA	C6-N1	2.45	1.43	1.38
3	A	2530	2MA	C2-N1	2.26	1.43	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	792	5MU	C5-C4-N3	12.67	126.12	115.31
3	A	1966	5MU	C5-C4-N3	12.42	125.91	115.31
3	A	792	5MU	C5-C6-N1	-10.70	112.34	123.34
3	A	1966	5MU	C5-C6-N1	-10.55	112.48	123.34
3	A	792	5MU	O4-C4-C5	-5.79	118.19	124.90
3	A	792	5MU	C4-N3-C2	-5.39	120.37	127.35
3	A	1966	5MU	C4-N3-C2	-5.00	120.87	127.35
3	A	1966	5MU	O4-C4-C5	-4.84	119.29	124.90
3	A	792	5MU	N3-C2-N1	4.69	121.11	114.89
3	A	1966	5MU	N3-C2-N1	4.27	120.56	114.89
3	A	1966	5MU	C5M-C5-C6	-4.08	117.40	122.85
3	A	1966	5MU	C5M-C5-C4	3.94	123.10	118.77
3	A	2530	2MA	C5-C6-N1	3.49	120.04	114.02
3	A	792	5MU	C5M-C5-C6	-3.38	118.34	122.85
3	A	2530	2MA	C8-N7-C5	2.99	108.69	102.99
3	A	2530	2MA	CM2-C2-N1	2.90	122.69	116.23
3	A	1966	5MU	O4-C4-N3	-2.77	114.80	120.12
3	A	792	5MU	C5M-C5-C4	2.67	121.71	118.77
3	A	1966	5MU	O2-C2-N1	-2.48	119.50	122.79
3	A	792	5MU	O2-C2-N1	-2.36	119.64	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	792	5MU	O4-C4-N3	-2.31	115.68	120.12
3	A	792	5MU	C6-C5-C4	2.30	119.95	118.03
3	A	792	5MU	C1'-N1-C2	2.11	121.40	117.57

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	792	5MU	C3'-C4'-C5'-O5'
3	A	792	5MU	O4'-C4'-C5'-O5'
3	A	2530	2MA	O4'-C4'-C5'-O5'
3	A	2530	2MA	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2530	2MA	1	0
3	A	792	5MU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

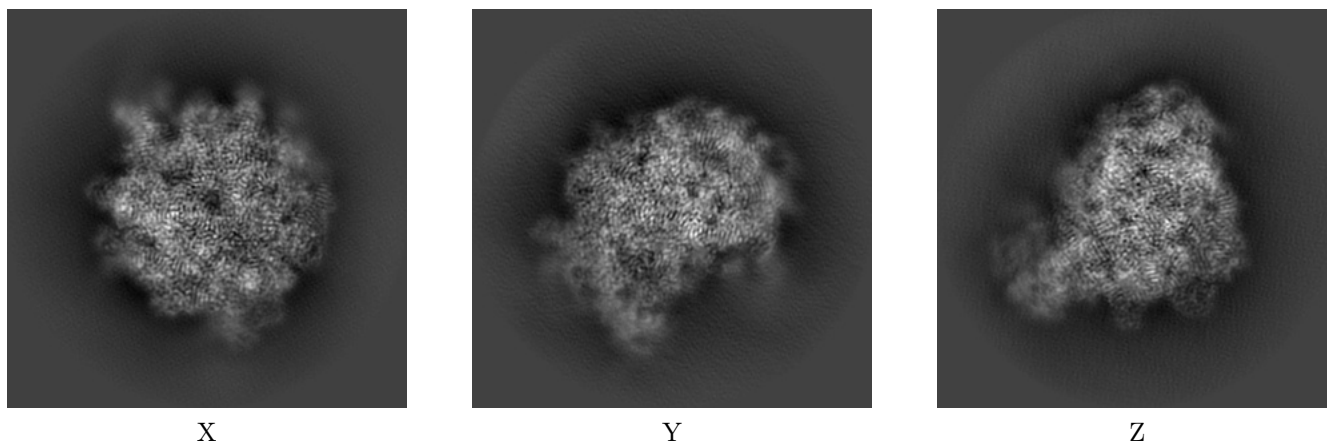
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11900. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

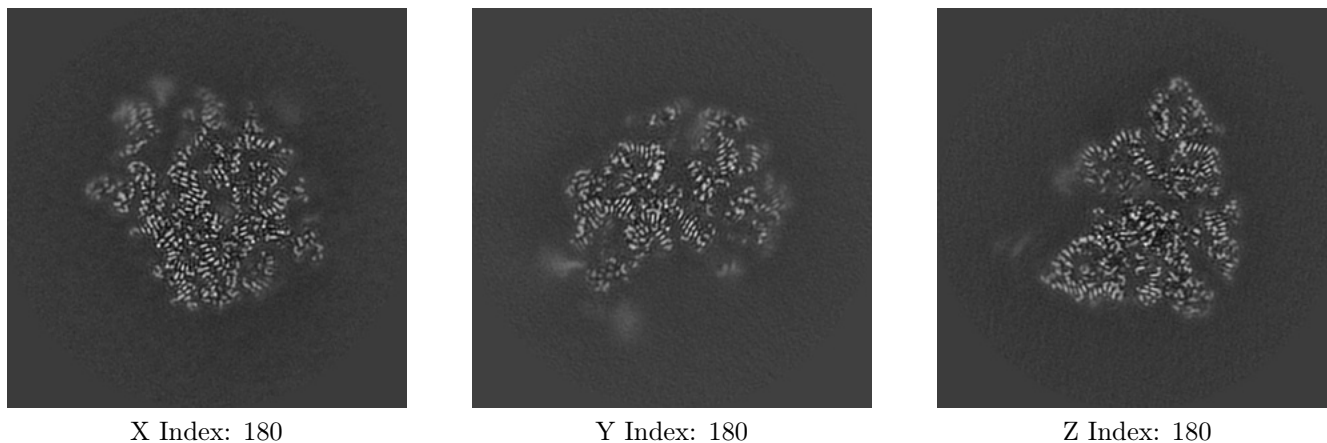
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

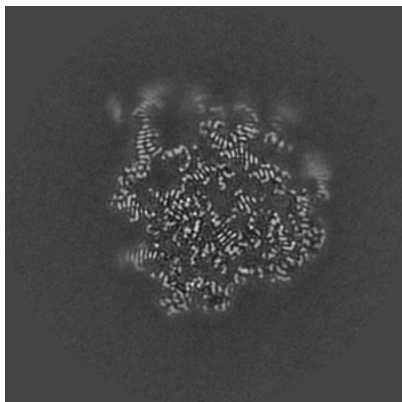
#### 6.2.1 Primary map



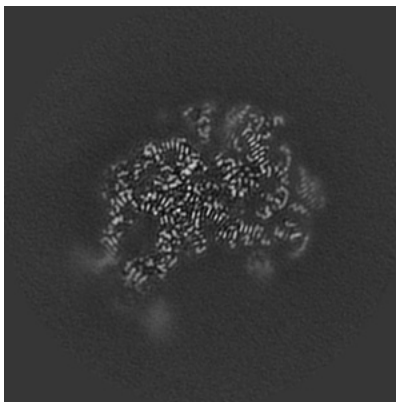
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

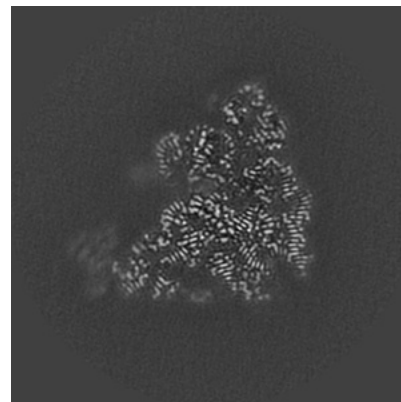
### 6.3.1 Primary map



X Index: 193



Y Index: 176

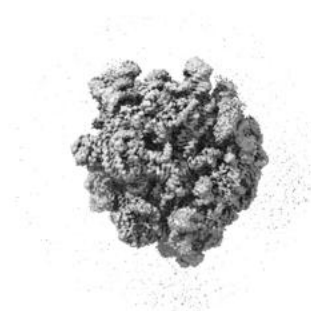


Z Index: 173

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

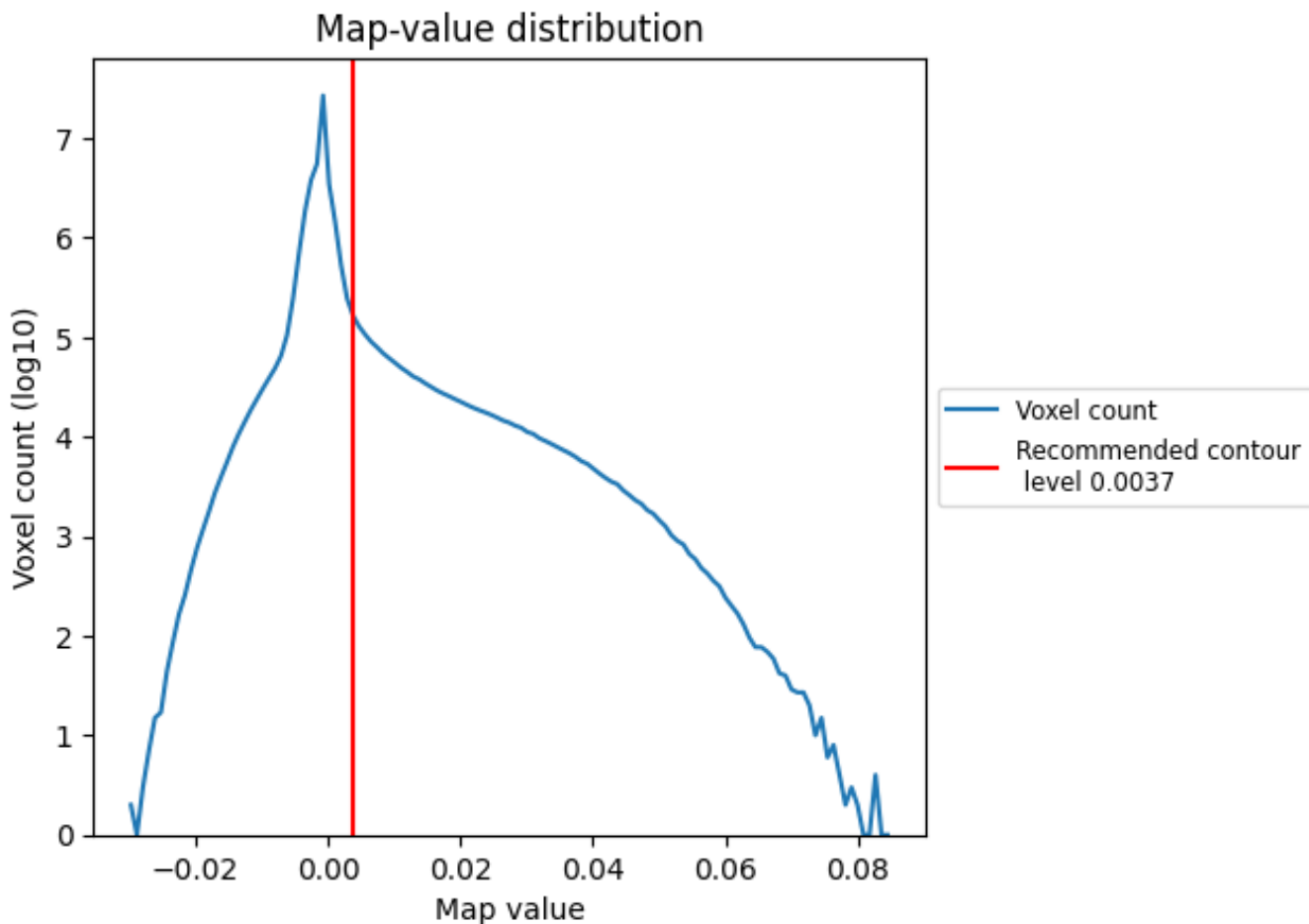
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

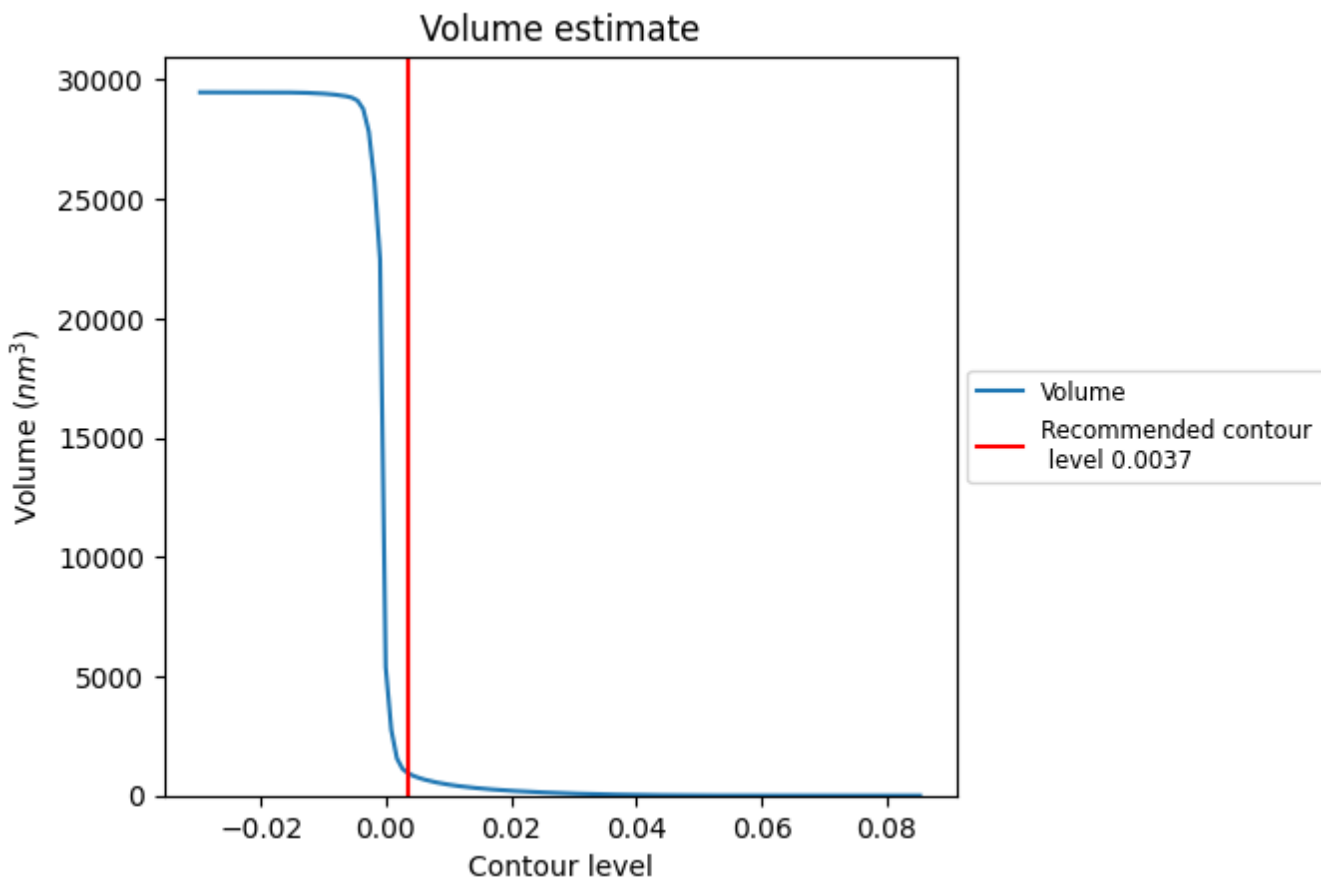
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

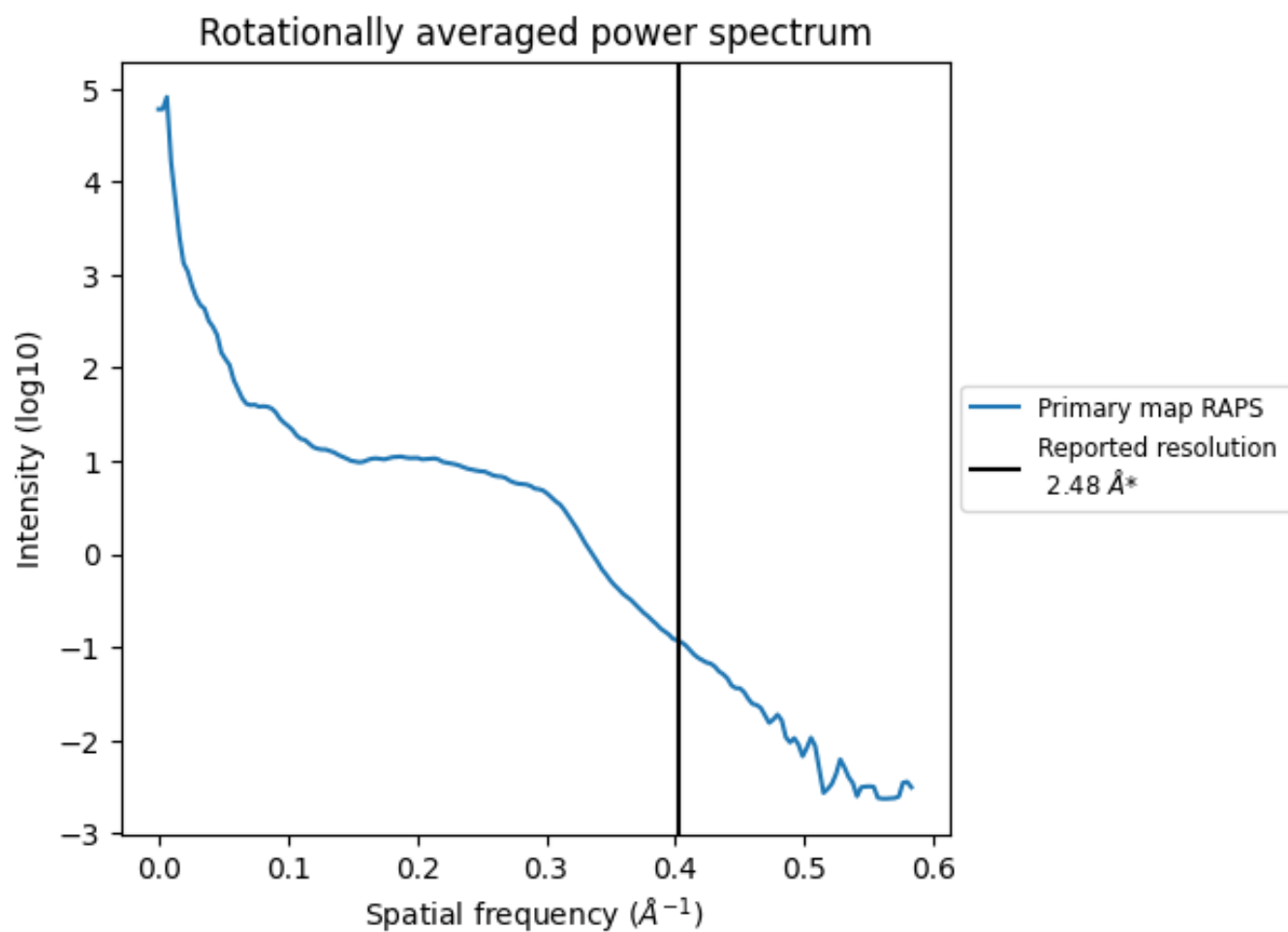


The volume at the recommended contour level is 916 nm<sup>3</sup>; this corresponds to an approximate mass of 827 kDa.

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 0.403 Å<sup>-1</sup>

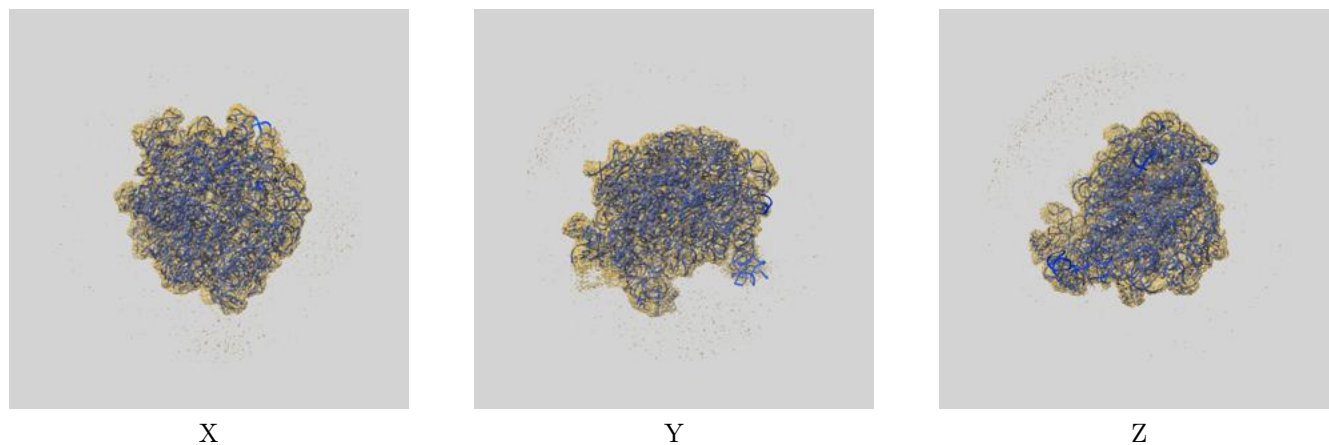
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

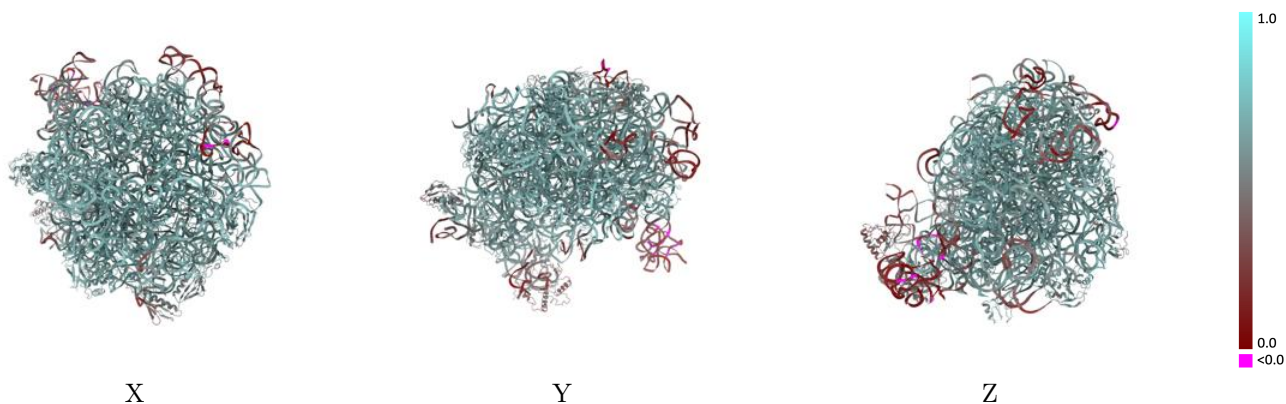
This section contains information regarding the fit between EMDB map EMD-11900 and PDB model 7ASM. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



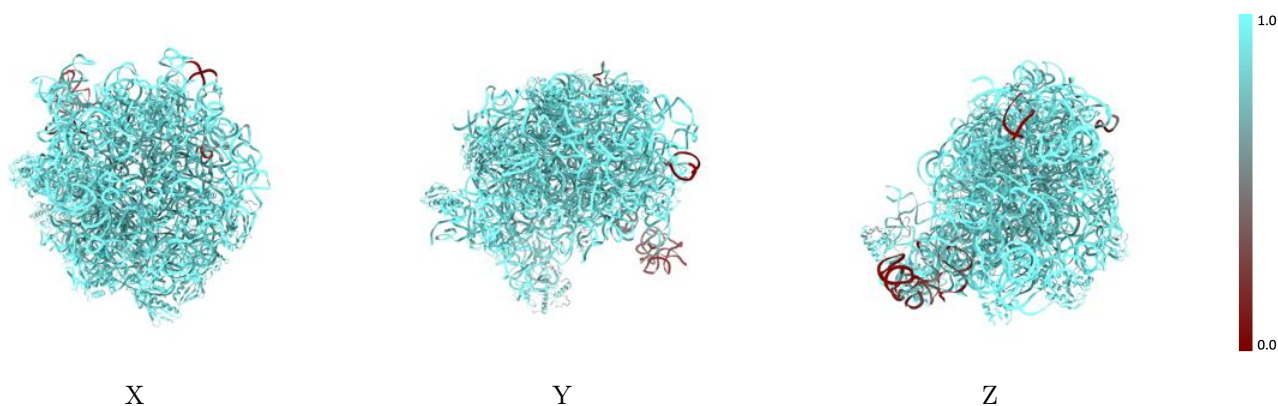
The images above show the 3D surface view of the map at the recommended contour level 0.0037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



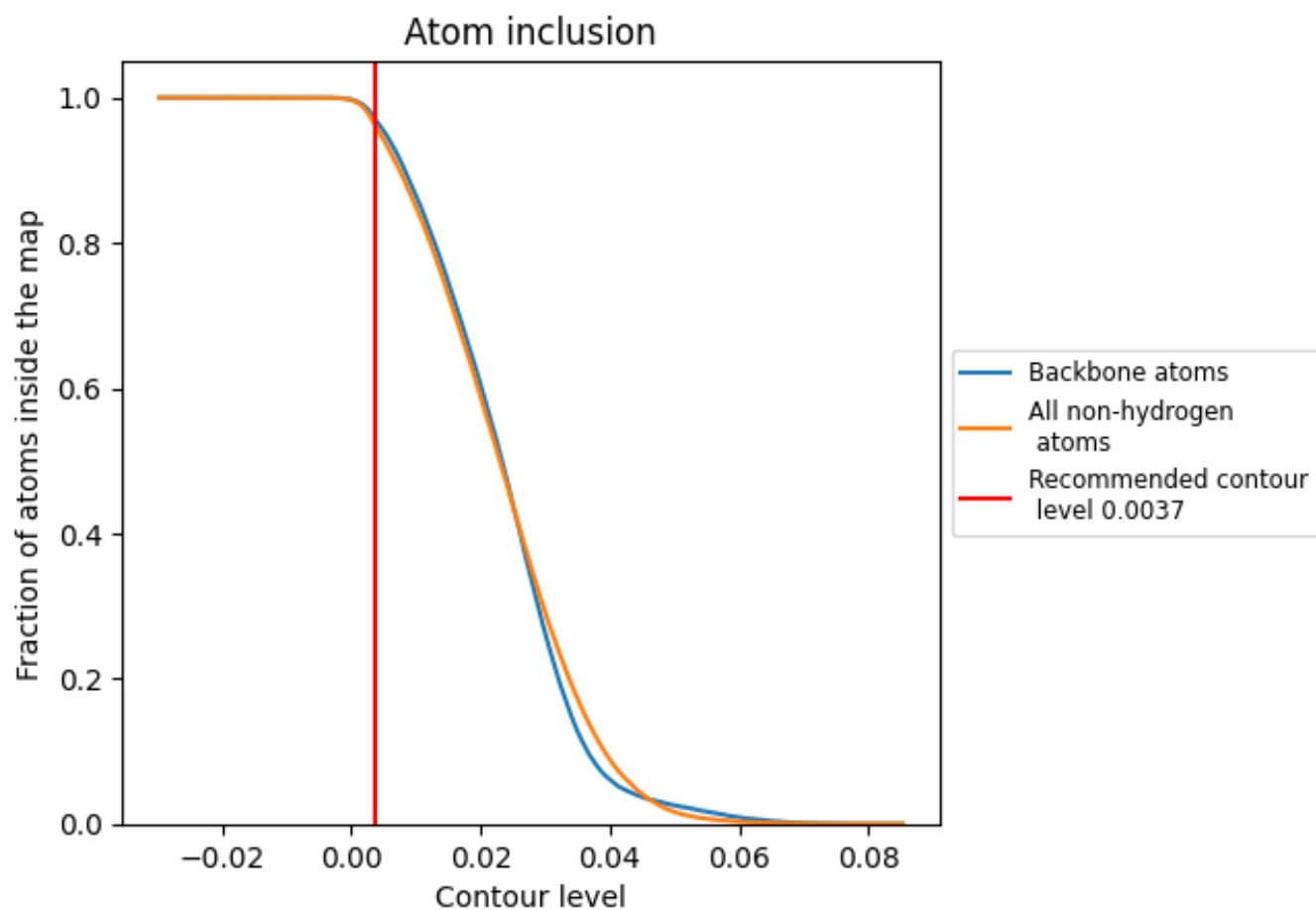
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0037).





























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.0037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9622	 0.6000
1	 0.7787	 0.5820
2	 0.9913	 0.6820
3	 0.9920	 0.6650
4	 0.9792	 0.6120
A	 0.9586	 0.5980
B	 0.9963	 0.5330
C	 0.9882	 0.6520
D	 0.9607	 0.6240
E	 0.9851	 0.6410
F	 0.8368	 0.3580
G	 0.9466	 0.5060
H	 0.9732	 0.6380
I	 0.9743	 0.6290
J	 0.9887	 0.6420
K	 0.9884	 0.6320
L	 0.9832	 0.6360
M	 0.9674	 0.5040
N	 0.9523	 0.6200
O	 0.9857	 0.6640
P	 0.9833	 0.6350
Q	 0.9820	 0.6610
R	 0.9757	 0.6230
S	 0.9759	 0.5770
T	 0.9661	 0.5790
U	 0.9810	 0.6460
V	 0.9781	 0.6060
W	 0.9638	 0.5910
X	 0.9773	 0.6380
Z	 0.9971	 0.6100

