



Full wwPDB EM Validation Report ⓘ

Jul 1, 2025 – 05:58 pm BST

PDB ID : 9H0L / pdb_00009h0l
EMDB ID : EMD-51758
Title : 70S ribosome with cognate tRNA^{Ser3} bound to A-site AGC codon
Authors : Akbar, S.; Larsson, D.S.D.; Selmer, M.
Deposited on : 2024-10-08
Resolution : 2.49 Å (reported)
Based on initial models : 8CGJ, 8CF1, 8CGK, 7K00

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 : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

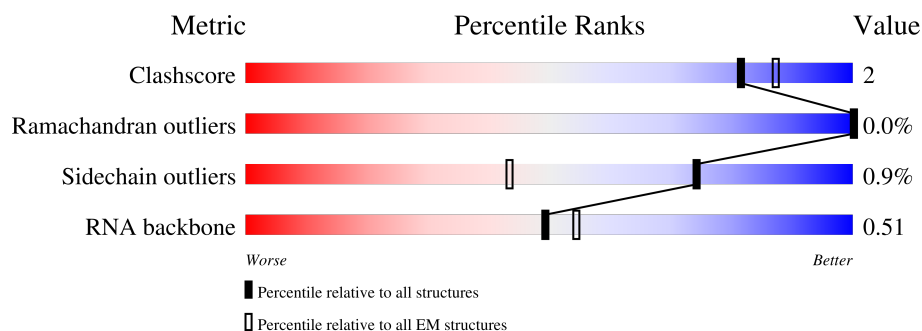
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.49 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.



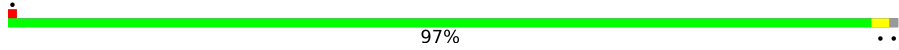
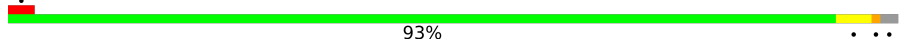


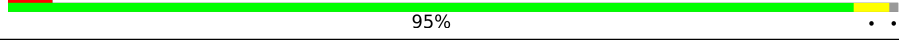
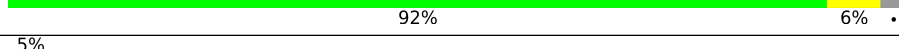
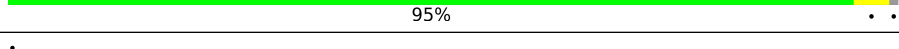
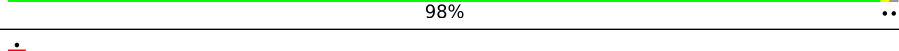
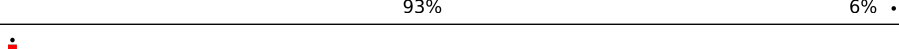
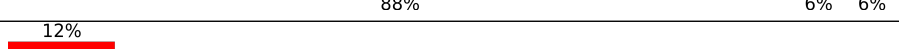
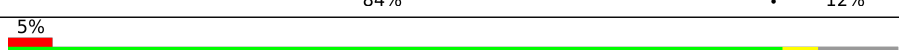

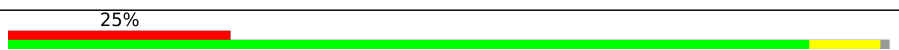
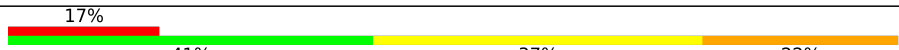
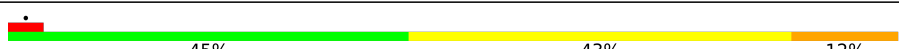




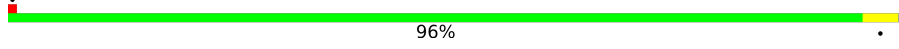
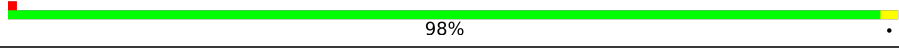
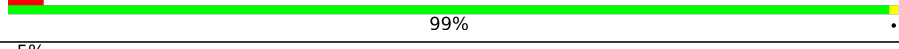

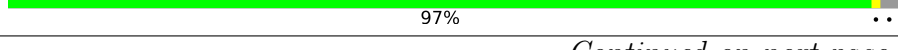

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1542	
2	B	241	
3	C	233	
4	D	206	
5	E	167	
6	F	135	
7	G	179	


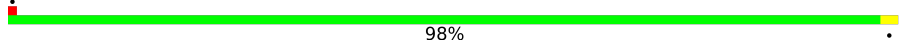
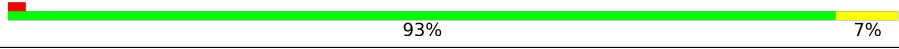
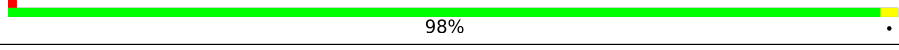
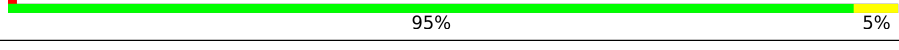
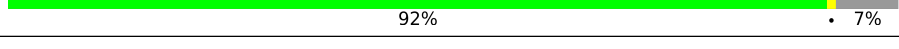

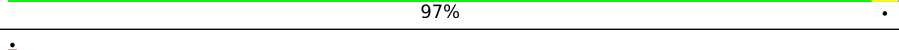
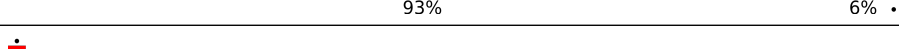
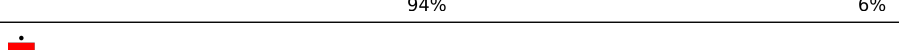
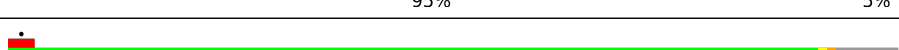
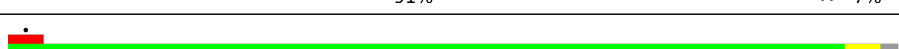

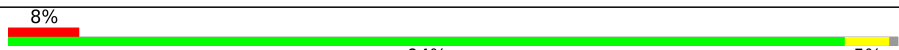
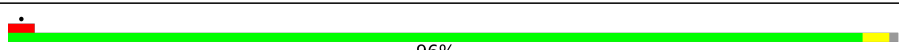

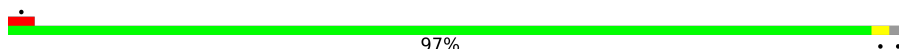
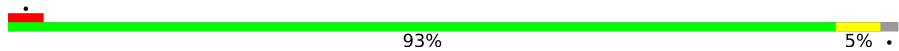
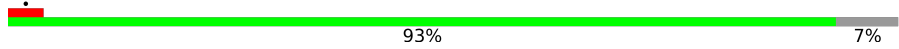
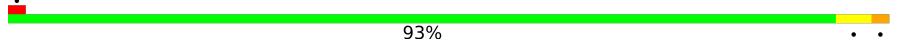
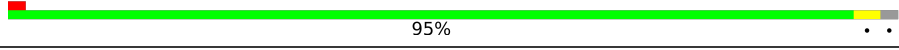



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Mol	Chain	Length	Quality of chain
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	V	76	
22	Z	76	
23	X	24	
24	Y	93	
25	a	2904	
26	b	120	
27	c	273	
28	d	209	
29	e	201	
30	f	179	
31	g	177	

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Mol	Chain	Length	Quality of chain
32	h	149	 28% 72%
33	i	142	 98%
34	j	123	 93% 7%
35	k	144	 98%
36	l	136	 95% 5%
37	m	127	 92% 7%
38	n	117	 85% 14% ..
39	o	115	 5% 97% ..
40	p	118	 93% 6%
41	q	103	 94% 6%
42	r	110	 95% 5%
43	s	100	 91% .. 7%
44	t	104	 94% ..
45	u	94	 99%
46	v	85	 8% 94% 5%
47	w	78	 96% ..
48	x	63	 90% 6%
49	y	59	 97% ..
50	z	57	 93% 5%
51	0	55	 93% 7%
52	1	46	 93% ..
53	2	65	 95% ..
54	3	38	 89% 11%
55	4	70	 10% 70% 16% 14%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 144192 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1529	Total	C	N	O	P	0	0
			32825	14647	6024	10625	1529		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

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

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

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

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

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

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

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

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

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

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

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

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

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

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

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

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

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

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

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

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 22 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		
22	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	11	Total	C	N	O	P	0	0
			240	108	50	71	11		

- Molecule 24 is a RNA chain called tRNA(Ser3).

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	Y	93	Total	C	N	O	P	S	0	0
			2000	893	365	648	92	2		

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 27 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 29 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 31 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	173	Total	C	N	O	S	0	0
			1295	814	237	242	2		

- Molecule 32 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 33 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 35 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 37 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 38 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 39 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	84	Total	C	N	O	S	0	0
			628	388	126	113	1		

- Molecule 47 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

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

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

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

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

- Molecule 51 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	0	51	Total	C	N	O	0	0
			417	269	76	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

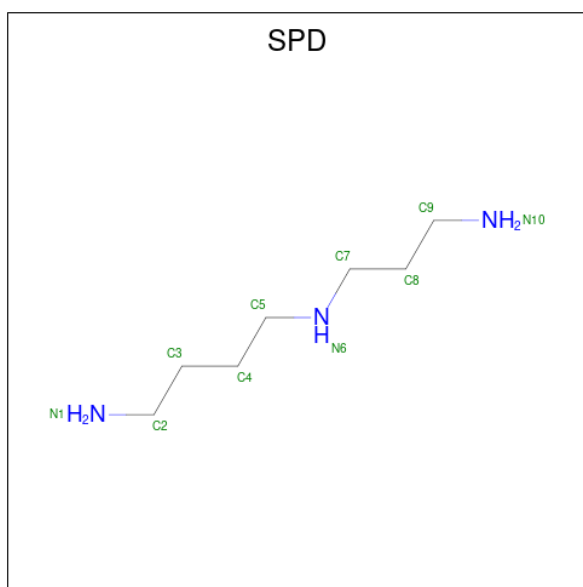
- Molecule 55 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

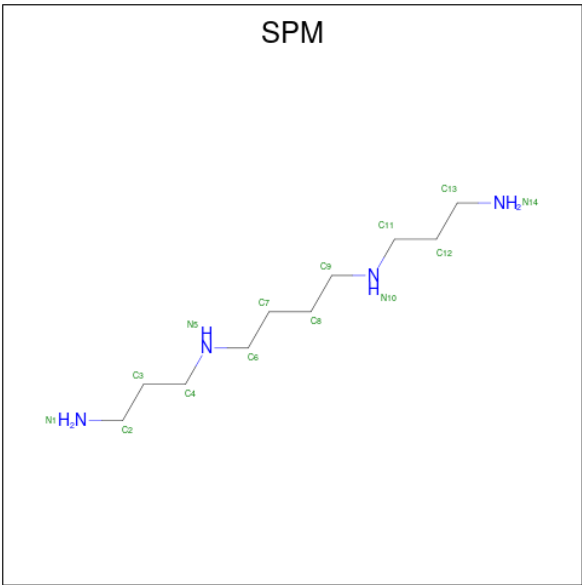
Mol	Chain	Residues	Atoms		AltConf
56	A	93	Total	Mg	0
			93	93	
56	Y	6	Total	Mg	0
			6	6	
56	a	206	Total	Mg	0
			206	206	
56	b	5	Total	Mg	0
			5	5	
56	c	1	Total	Mg	0
			1	1	
56	d	1	Total	Mg	0
			1	1	
56	m	1	Total	Mg	0
			1	1	
56	z	1	Total	Mg	0
			1	1	

- Molecule 57 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



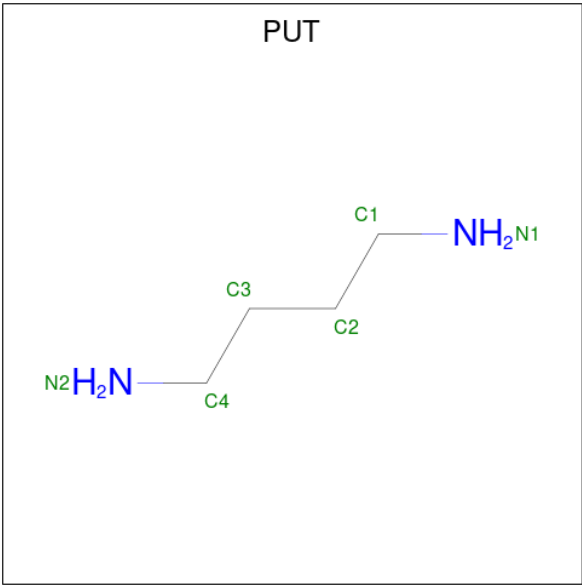
Mol	Chain	Residues	Atoms			AltConf
57	a	1	Total	C	N	0
			10	7	3	
57	a	1	Total	C	N	0
			10	7	3	
57	a	1	Total	C	N	0
			10	7	3	
57	a	1	Total	C	N	0
			10	7	3	
57	a	1	Total	C	N	0
			10	7	3	

- Molecule 58 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
58	a	1	Total	C	N	0
			14	10	4	

- Molecule 59 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	

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Mol	Chain	Residues	Atoms			AltConf
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	
59	a	1	Total	C	N	0
			6	4	2	

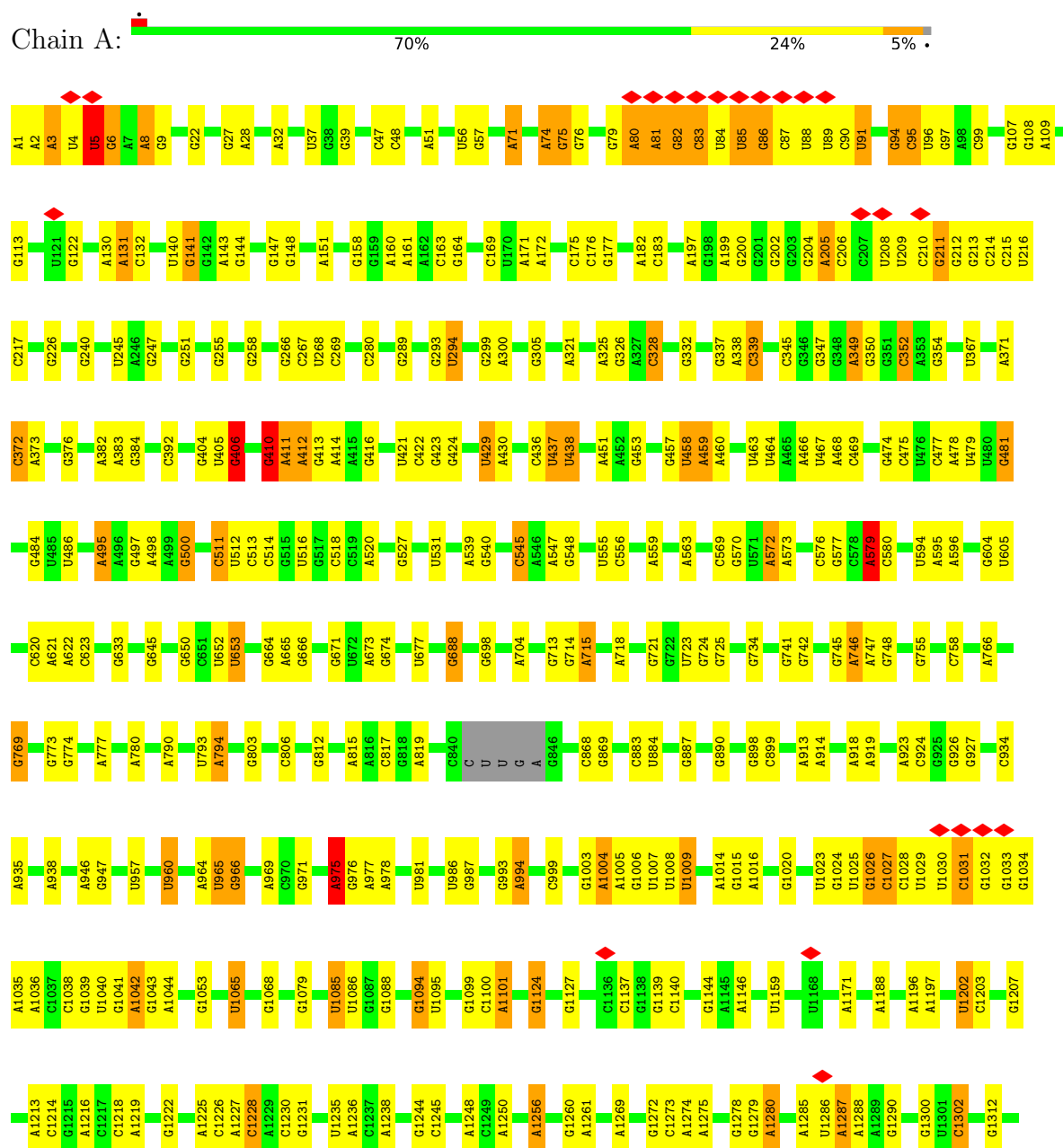
- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

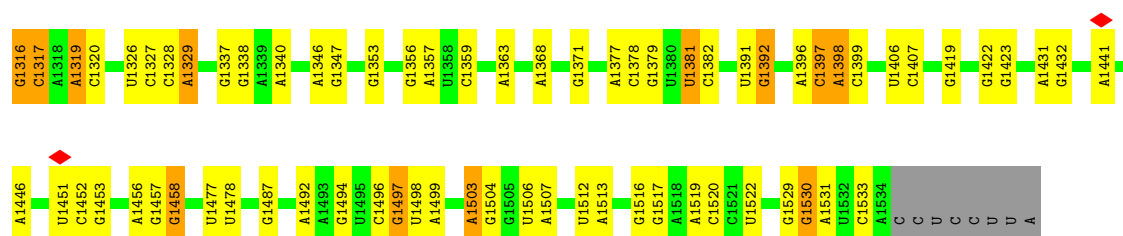
Mol	Chain	Residues	Atoms		AltConf
60	3	1	Total	Zn	0
			1	1	
60	4	1	Total	Zn	0
			1	1	

3 Residue-property plots

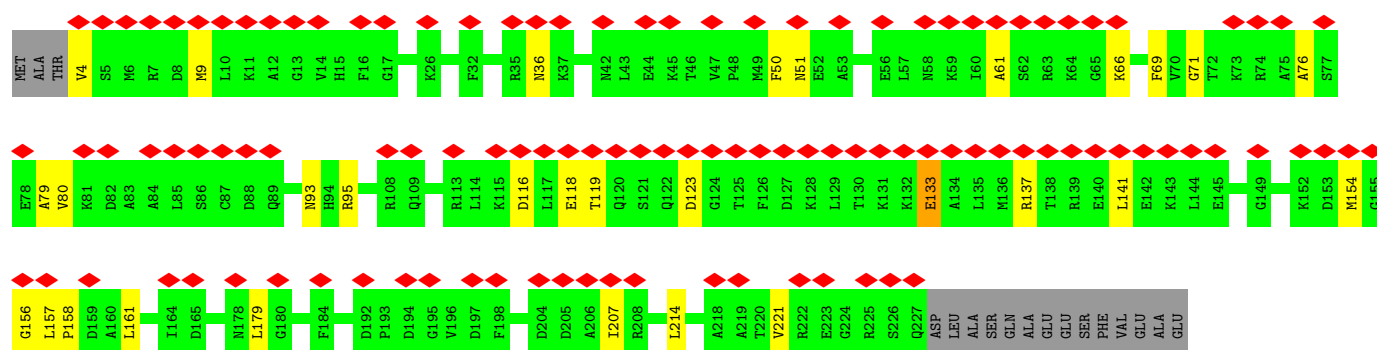
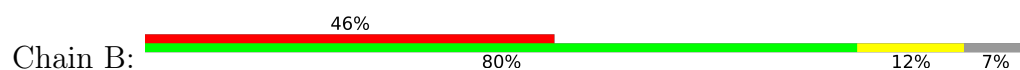
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

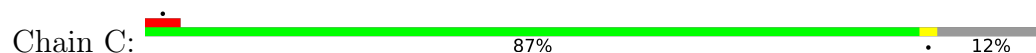




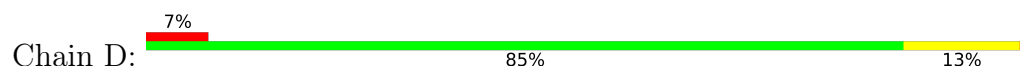
• Molecule 2: Small ribosomal subunit protein uS2



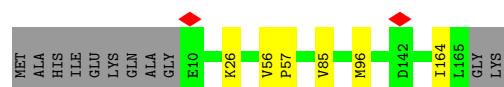
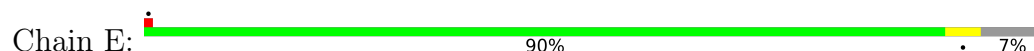
• Molecule 3: Small ribosomal subunit protein uS3



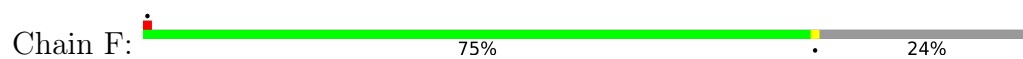
• Molecule 4: Small ribosomal subunit protein uS4



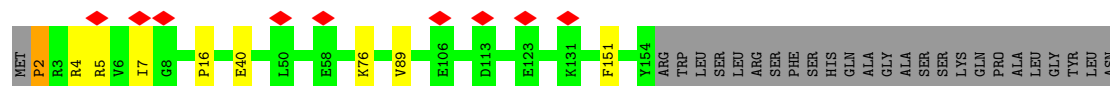
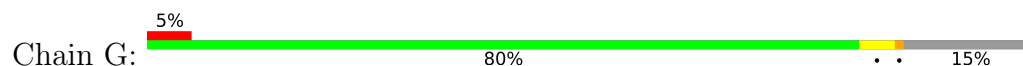
• Molecule 5: Small ribosomal subunit protein uS5



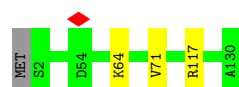
• Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform



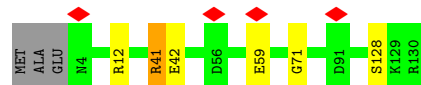
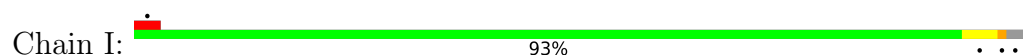
- Molecule 7: Small ribosomal subunit protein uS7



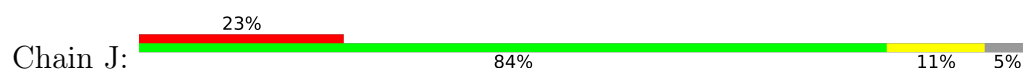
- Molecule 8: Small ribosomal subunit protein uS8



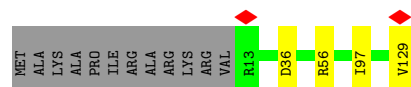
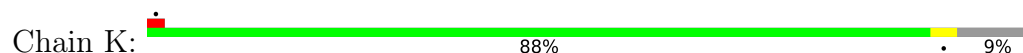
- Molecule 9: Small ribosomal subunit protein uS9



- Molecule 10: Small ribosomal subunit protein uS10

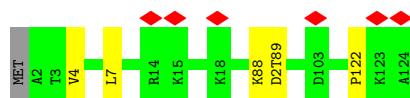


- Molecule 11: Small ribosomal subunit protein uS11

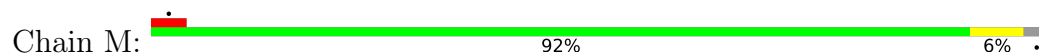


- Molecule 12: Small ribosomal subunit protein uS12

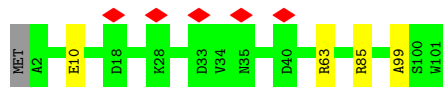




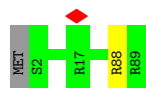
- Molecule 13: Small ribosomal subunit protein uS13



- Molecule 14: Small ribosomal subunit protein uS14



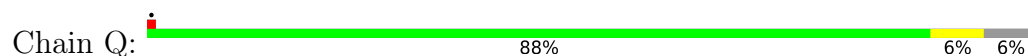
- Molecule 15: Small ribosomal subunit protein uS15



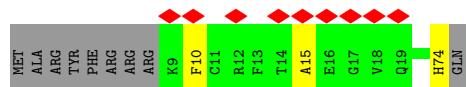
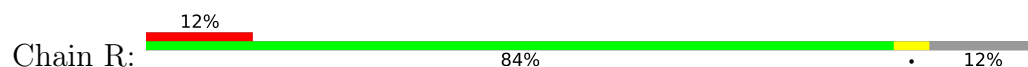
- Molecule 16: Small ribosomal subunit protein bS16



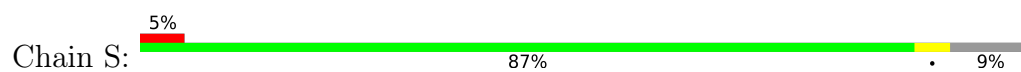
- Molecule 17: Small ribosomal subunit protein uS17



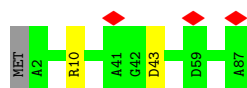
- Molecule 18: Small ribosomal subunit protein bS18



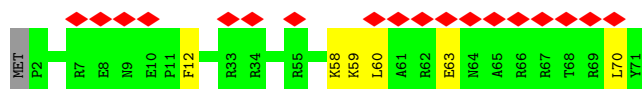
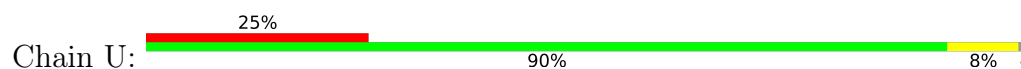
- Molecule 19: Small ribosomal subunit protein uS19



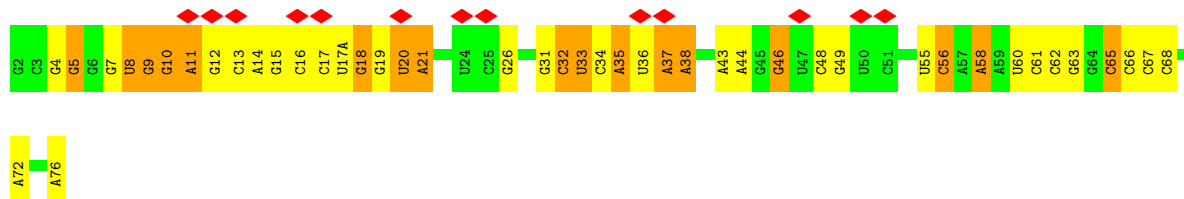
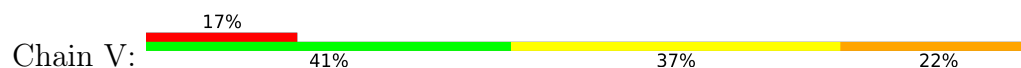
- Molecule 20: Small ribosomal subunit protein bS20



- Molecule 21: Small ribosomal subunit protein bS21



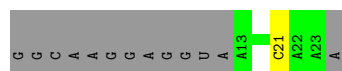
- Molecule 22: tRNA(fMet)



- Molecule 22: tRNA(fMet)

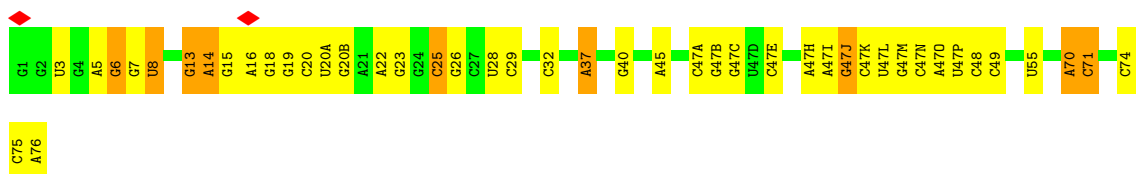


- Molecule 23: mRNA



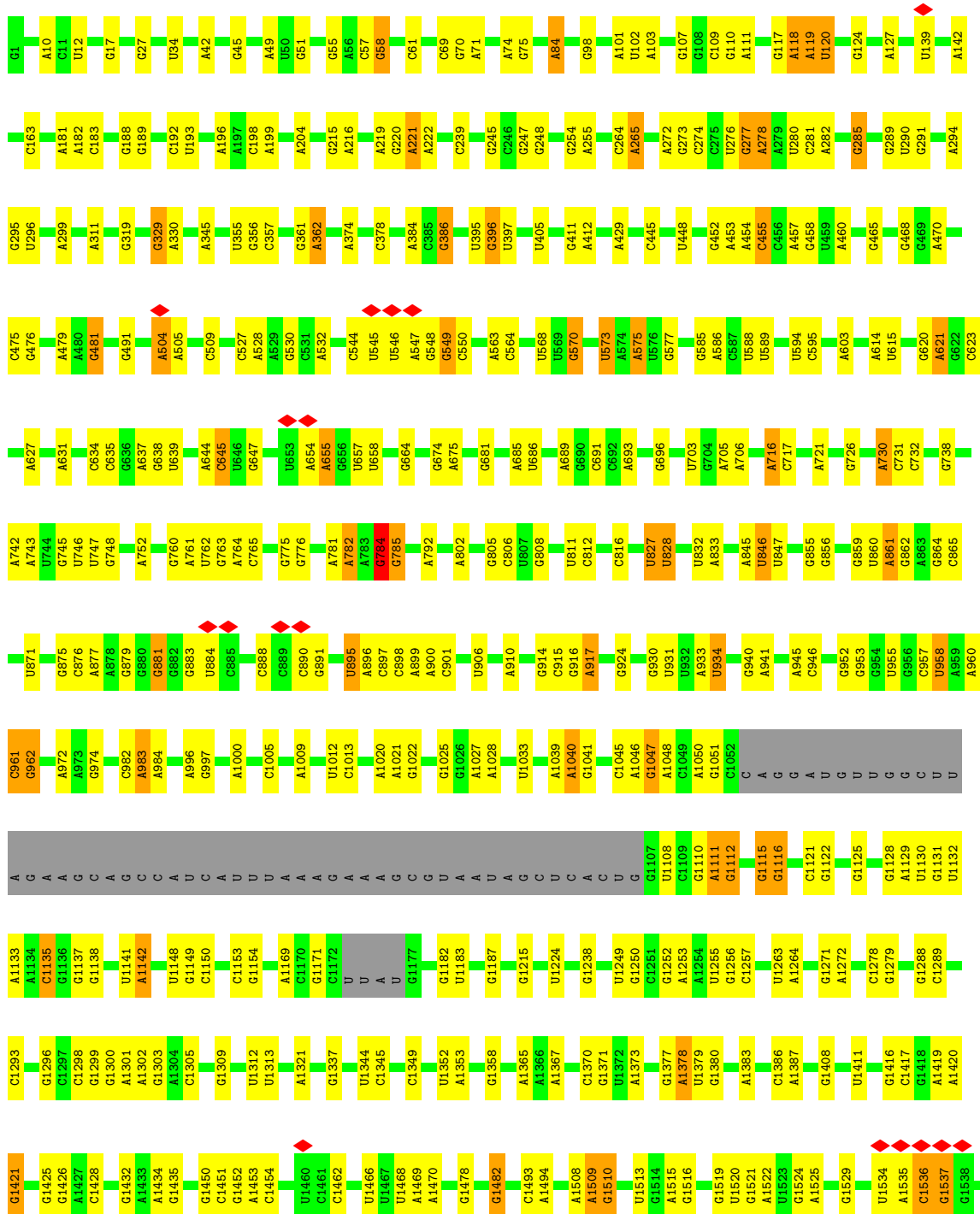
- Molecule 24: tRNA(Ser3)

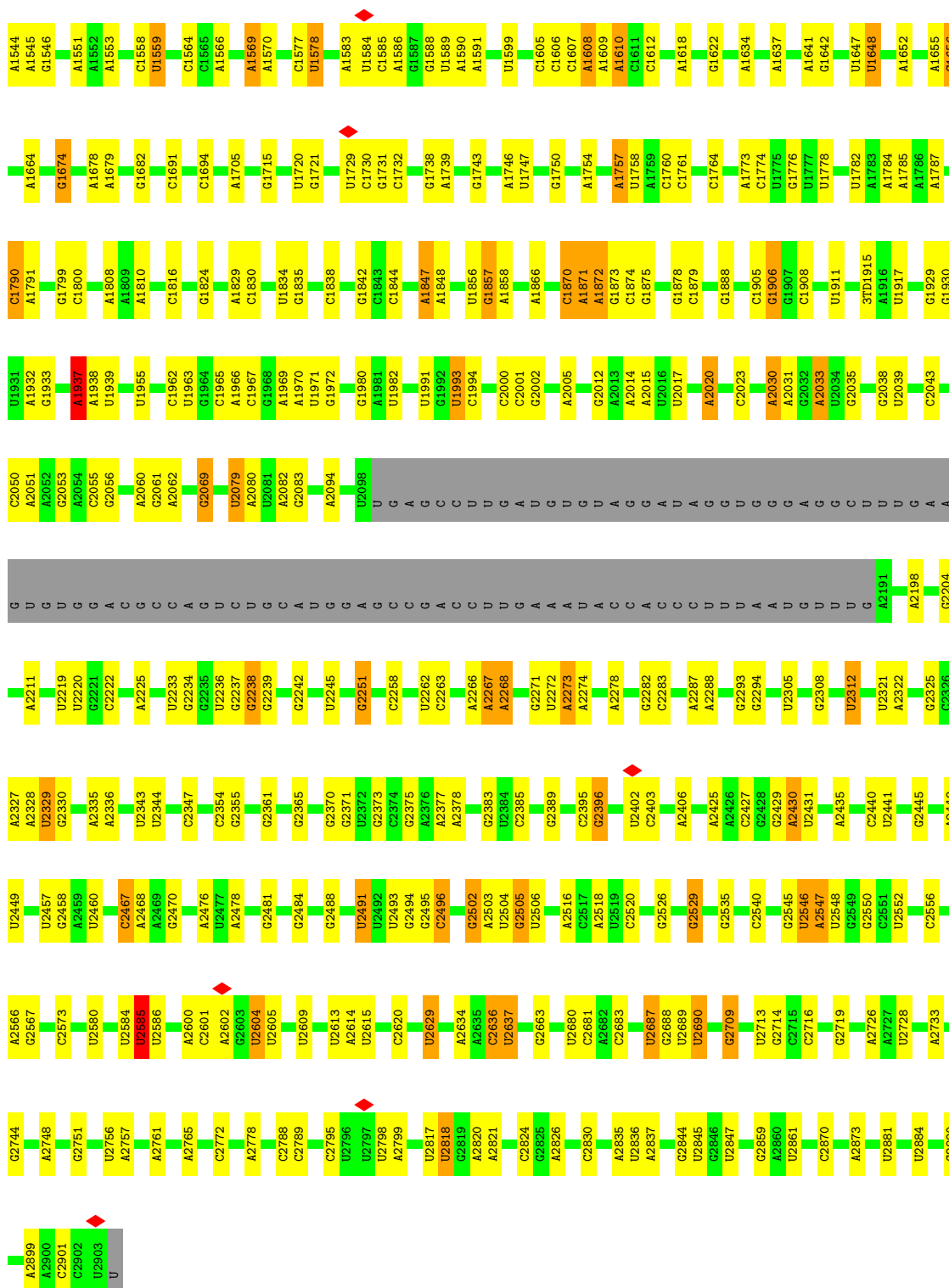




Molecule 25: 23S rRNA

Chain a: 68% 23% 5%





- Molecule 27: Large ribosomal subunit protein uL2

Chain c:  96%



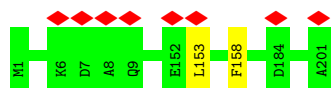
- Molecule 28: Large ribosomal subunit protein uL3

Chain d:  98%




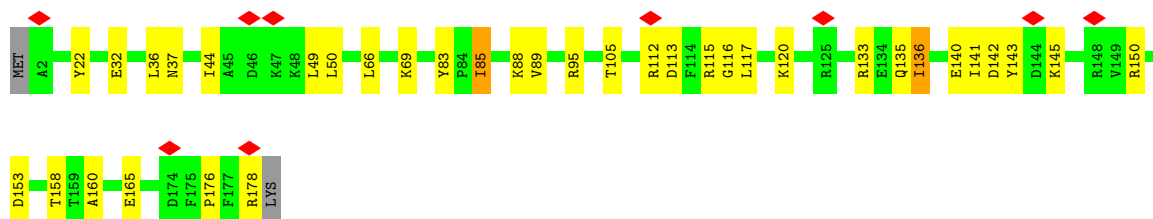
- Molecule 29: Large ribosomal subunit protein uL4

Chain e:  99%



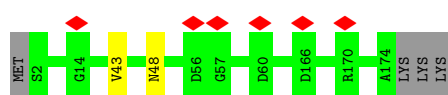
- Molecule 30: Large ribosomal subunit protein uL5

Chain f:  5% 79% 19%



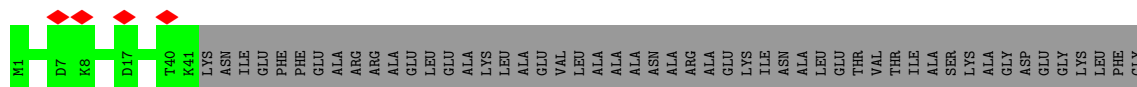
- Molecule 31: Large ribosomal subunit protein uL6

Chain g:  97%



- Molecule 32: Large ribosomal subunit protein bL9

Chain h:  28% 72%



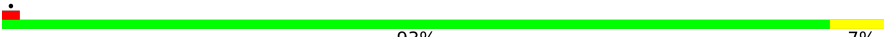
SER
ILE
GLY
THR
ARG
ASP
TLE
ALA
ASP
ALA
VAL
THR
ALA
ALA
GLY
VAL
GLU
VAL
ALA
LYS
SER
GLU
VAL
ARG
LEU
PRO
ASN
GLY
VAL
LEU
ARG
THR
THR
GLY
GLU
HIS
GLU
VAL
SER
PHE
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PHE
ALA
LYS
VAL
TLE
VAL
ASN
VAL
ALA
GLU

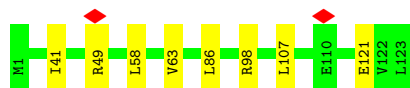
- Molecule 33: Large ribosomal subunit protein uL13

Chain i:  98%



- Molecule 34: Large ribosomal subunit protein uL14

Chain j:  93%



- Molecule 35: Large ribosomal subunit protein uL15

Chain k:  98%



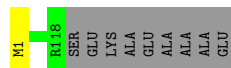
- Molecule 36: Large ribosomal subunit protein uL16

Chain l:  95%




- Molecule 37: Large ribosomal subunit protein bL17

Chain m:  92%



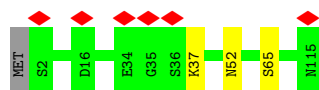
- Molecule 38: Large ribosomal subunit protein uL18

Chain n:  85%



- Molecule 39: Large ribosomal subunit protein bL19

Chain o:  97%



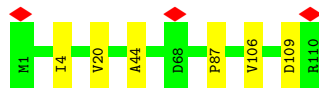
- Molecule 40: Large ribosomal subunit protein bL20



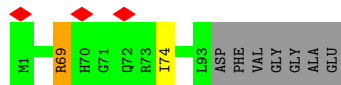
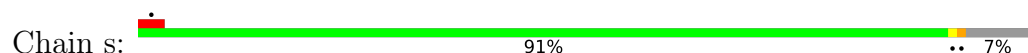
- Molecule 41: Large ribosomal subunit protein bL21



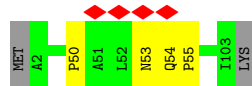
- Molecule 42: Large ribosomal subunit protein uL22



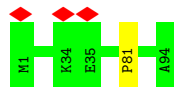
- Molecule 43: Large ribosomal subunit protein uL23



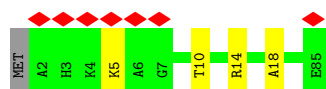
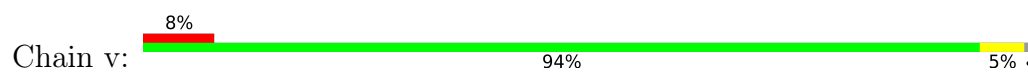
- Molecule 44: Large ribosomal subunit protein uL24



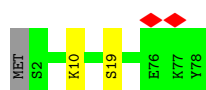
- Molecule 45: Large ribosomal subunit protein bL25



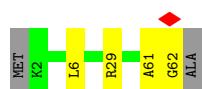
- Molecule 46: Large ribosomal subunit protein bL27



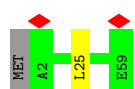
- Molecule 47: Large ribosomal subunit protein bL28



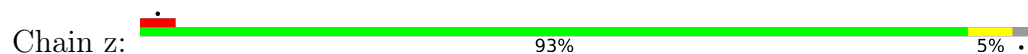
- Molecule 48: Large ribosomal subunit protein uL29



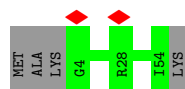
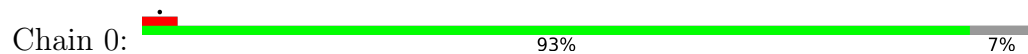
- Molecule 49: Large ribosomal subunit protein uL30



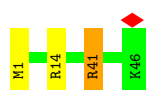
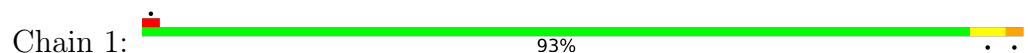
- Molecule 50: Large ribosomal subunit protein bL32



- Molecule 51: Large ribosomal subunit protein bL33



- Molecule 52: Large ribosomal subunit protein bL34




- Molecule 53: Large ribosomal subunit protein bL35

Chain 2:  95%



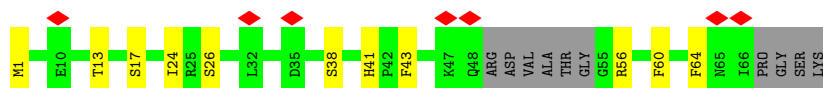
- Molecule 54: Large ribosomal subunit protein bL36A

Chain 3:  89% 11%



- Molecule 55: Large ribosomal subunit protein bL31A

Chain 4:  10% 70% 16% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	167986	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28.5	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.632	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	382.1056, 382.1056, 382.1056	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7463, 0.7463, 0.7463	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 1MG, T6A, 2MA, MG, RSP, G7M, 5MC, PSU, IAS, UR3, D2T, PUT, SPM, H2U, 4OC, SPD, MS6, 6MZ, OMU, MEQ, MA6, 4SU, OMG, ZN, 2MG, 5MU, OMC, 4D4

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	0.55	1/36475 (0.0%)	0.99	84/56895 (0.1%)
2	B	0.54	0/1784	1.08	5/2403 (0.2%)
3	C	0.52	0/1651	0.94	0/2225
4	D	0.50	0/1665	1.01	0/2227
5	E	0.58	0/1165	1.00	2/1568 (0.1%)
6	F	0.52	0/858	0.90	0/1160
7	G	0.52	0/1219	0.97	0/1635
8	H	0.53	0/989	0.93	0/1326
9	I	0.54	0/1034	1.01	1/1375 (0.1%)
10	J	0.53	0/796	0.98	0/1077
11	K	0.60	0/884	0.94	1/1191 (0.1%)
12	L	0.60	0/960	0.99	1/1286 (0.1%)
13	M	0.53	0/900	1.01	0/1204
14	N	0.54	0/817	0.98	0/1088
15	O	0.53	0/722	0.96	0/964
16	P	0.52	0/653	0.92	1/877 (0.1%)
17	Q	0.53	0/650	0.93	0/871
18	R	0.56	0/553	0.99	0/742
19	S	0.55	0/685	0.94	0/922
20	T	0.53	0/676	1.03	0/895
21	U	0.54	0/597	1.00	0/792
22	V	0.59	0/1813	0.83	0/2825
22	Z	0.58	0/1813	0.88	1/2825 (0.0%)
23	X	0.58	0/270	1.06	1/419 (0.2%)
24	Y	0.59	1/2088 (0.0%)	0.82	0/3255
25	a	0.58	1/65651 (0.0%)	1.10	275/102413 (0.3%)
26	b	0.58	0/2850	1.01	7/4444 (0.2%)
27	c	0.67	1/2121 (0.0%)	1.06	1/2852 (0.0%)
28	d	0.61	0/1576	0.98	1/2119 (0.0%)
29	e	0.56	0/1571	1.00	0/2113
30	f	0.47	0/1434	0.81	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	g	0.52	0/1315	0.94	0/1783
32	h	0.56	0/306	0.98	0/413
33	i	0.58	0/1152	0.98	0/1551
34	j	0.57	0/955	1.00	0/1279
35	k	0.59	0/1062	1.01	0/1413
36	l	0.60	0/1073	0.98	0/1433
37	m	0.64	0/958	1.03	1/1281 (0.1%)
38	n	0.54	0/902	0.88	0/1209
39	o	0.55	0/929	0.95	0/1242
40	p	0.59	0/960	1.04	2/1278 (0.2%)
41	q	0.56	0/829	0.94	0/1107
42	r	0.60	0/864	0.98	0/1156
43	s	0.55	0/744	0.98	0/994
44	t	0.51	0/787	0.90	0/1051
45	u	0.56	0/766	0.96	0/1025
46	v	0.65	0/636	0.97	0/841
47	w	0.59	0/635	1.00	0/848
48	x	0.47	0/496	0.98	0/660
49	y	0.57	0/453	0.98	0/605
50	z	0.67	0/450	1.04	1/599 (0.2%)
51	0	0.53	0/424	0.92	0/565
52	1	0.66	0/380	1.16	1/498 (0.2%)
53	2	0.66	0/513	1.06	0/676
54	3	0.56	0/303	0.98	0/397
55	4	0.51	0/488	0.77	0/649
All	All	0.57	4/155300 (0.0%)	1.03	386/232467 (0.2%)

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
4	D	0	1
8	H	0	1
9	I	0	1
10	J	0	2
13	M	0	1
14	N	0	1
33	i	0	1
40	p	0	2
41	q	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	s	0	1
46	v	0	1
48	x	0	1
52	1	0	1
53	2	0	1
54	3	0	1
All	All	0	17

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	53	HIS	CG-CD2	-6.15	1.29	1.35
25	a	2069	G7M	O3'-P	5.49	1.61	1.56
24	Y	8	4SU	O3'-P	5.29	1.61	1.56
1	A	1498	UR3	O3'-P	5.09	1.61	1.56

All (386) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	1648	U	O3'-P-O5'	-11.09	87.37	104.00
25	a	2263	C	O3'-P-O5'	-9.82	89.26	104.00
25	a	917	A	O3'-P-O5'	-9.30	90.05	104.00
25	a	1131	G	O3'-P-O5'	-9.28	90.09	104.00
25	a	2079	U	O3'-P-O5'	-9.16	90.26	104.00
25	a	1810	A	O3'-P-O5'	-9.15	90.27	104.00
25	a	731	C	O3'-P-O5'	-9.14	90.29	104.00
25	a	1937	A	O3'-P-O5'	-9.03	90.45	104.00
25	a	329	G	O3'-P-O5'	-8.98	90.53	104.00
25	a	1776	G	O3'-P-O5'	-8.87	90.69	104.00
25	a	2002	G	O3'-P-O5'	-8.74	90.89	104.00
25	a	760	G	O3'-P-O5'	-8.54	91.19	104.00
25	a	2278	A	O3'-P-O5'	-8.53	91.21	104.00
25	a	2222	C	O3'-P-O5'	-8.43	91.35	104.00
25	a	1551	A	O3'-P-O5'	-8.28	91.57	104.00
25	a	2614	A	O3'-P-O5'	-8.12	91.82	104.00
25	a	2262	U	O3'-P-O5'	-8.11	91.84	104.00
25	a	2881	U	O3'-P-O5'	-8.04	91.93	104.00
25	a	2001	C	O3'-P-O5'	-7.95	92.08	104.00
25	a	1313	U	C2'-C3'-O3'	-7.93	101.80	113.70
25	a	827	U	C1'-C2'-O2'	-7.86	96.61	108.40
25	a	726	G	O3'-P-O5'	-7.76	92.35	104.00
25	a	1656	C	C1'-C2'-O2'	-7.75	96.77	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	1137	G	O3'-P-O5'	-7.75	92.37	104.00
25	a	2493	U	O3'-P-O5'	-7.74	92.38	104.00
25	a	1312	U	O3'-P-O5'	-7.72	92.43	104.00
25	a	1468	U	O3'-P-O5'	-7.68	92.48	104.00
25	a	1844	C	O3'-P-O5'	-7.66	92.50	104.00
25	a	204	A	O3'-P-O5'	-7.65	92.53	104.00
25	a	2826	A	O3'-P-O5'	-7.64	92.54	104.00
25	a	1674	G	O3'-P-O5'	-7.62	92.57	104.00
25	a	1790	C	C2'-C3'-O3'	-7.61	102.29	113.70
2	B	141	LEU	CA-C-N	-7.47	108.25	120.72
2	B	141	LEU	C-N-CA	-7.47	108.25	120.72
25	a	2890	G	O3'-P-O5'	-7.34	92.99	104.00
25	a	730	A	O3'-P-O5'	-7.32	93.02	104.00
25	a	808	G	O3'-P-O5'	-7.31	93.04	104.00
1	A	548	G	O3'-P-O5'	-7.24	93.13	104.00
25	a	2268	A	O3'-P-O5'	7.24	114.85	104.00
25	a	972	A	O3'-P-O5'	-7.22	93.17	104.00
25	a	1373	A	O3'-P-O5'	-7.17	93.24	104.00
1	A	545	C	O3'-P-O5'	-7.14	93.29	104.00
25	a	2378	A	O3'-P-O5'	-7.14	93.29	104.00
25	a	2636	C	O3'-P-O5'	-7.11	93.34	104.00
25	a	17	G	O3'-P-O5'	-7.04	93.44	104.00
25	a	575	A	O3'-P-O5'	-7.03	93.45	104.00
25	a	1302	A	O3'-P-O5'	-7.00	93.50	104.00
25	a	1838	C	C1'-C2'-O2'	-7.00	101.31	111.80
25	a	2584	U	O3'-P-O5'	-6.99	93.52	104.00
1	A	769	G	O3'-P-O5'	-6.93	93.60	104.00
25	a	2830	C	C4'-C3'-C2'	-6.93	95.67	102.60
25	a	221	A	O3'-P-O5'	-6.90	93.65	104.00
1	A	328	C	O3'-P-O5'	-6.89	93.67	104.00
25	a	828	U	C4'-C3'-O3'	-6.88	102.67	113.00
9	I	128	SER	O-C-N	-6.84	115.19	123.27
25	a	1610	A	C1'-C2'-O2'	-6.84	101.55	111.80
1	A	938	A	O3'-P-O5'	-6.81	93.78	104.00
25	a	1278	C	O3'-P-O5'	-6.80	93.79	104.00
1	A	898	G	C1'-C2'-O2'	6.80	118.60	108.40
25	a	871	U	O3'-P-O5'	-6.79	93.81	104.00
25	a	1655	A	O3'-P-O5'	-6.79	93.81	104.00
25	a	2495	G	O3'-P-O5'	-6.73	93.91	104.00
25	a	861	A	O3'-P-O5'	-6.72	93.92	104.00
1	A	1377	A	O3'-P-O5'	-6.70	93.95	104.00
25	a	781	A	O3'-P-O5'	-6.66	94.01	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	254	G	O3'-P-O5'	-6.65	94.03	104.00
25	a	1025	G	O3'-P-O5'	6.64	113.96	104.00
1	A	520	A	O3'-P-O5'	-6.63	94.05	104.00
25	a	2272	U	C2'-C3'-O3'	-6.62	103.77	113.70
25	a	2481	G	C4'-C3'-O3'	-6.62	103.08	113.00
26	b	28	C	O3'-P-O5'	-6.61	94.08	104.00
25	a	1367	A	O3'-P-O5'	-6.59	94.11	104.00
25	a	2873	A	C1'-C2'-O2'	-6.59	101.91	111.80
25	a	906	U	O3'-P-O5'	-6.59	94.12	104.00
25	a	457	A	O3'-P-O5'	-6.58	94.12	104.00
25	a	1249	U	C1'-C2'-O2'	6.57	118.25	108.40
25	a	1377	G	O3'-P-O5'	-6.56	94.16	104.00
25	a	1757	A	C4'-C3'-O3'	-6.54	103.19	113.00
25	a	961	C	C1'-C2'-O2'	-6.53	102.00	111.80
25	a	2728	U	O3'-P-O5'	-6.53	94.20	104.00
25	a	384	A	C2'-C3'-O3'	-6.53	103.91	113.70
2	B	69	PHE	CA-C-N	-6.53	114.23	123.11
2	B	69	PHE	C-N-CA	-6.53	114.23	123.11
16	P	23	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	812	G	O3'-P-O5'	-6.48	94.29	104.00
25	a	1408	G	O3'-P-O5'	-6.47	94.30	104.00
25	a	1000	A	C1'-C2'-O2'	-6.43	98.75	108.40
25	a	504	A	O3'-P-O5'	-6.42	94.37	104.00
1	A	964	A	O3'-P-O5'	-6.41	94.38	104.00
1	A	1188	A	O3'-P-O5'	-6.39	94.41	104.00
25	a	2005	A	C2'-C3'-O3'	-6.38	104.12	113.70
26	b	14	U	O3'-P-O5'	-6.36	94.45	104.00
1	A	913	A	O3'-P-O5'	-6.36	94.46	104.00
1	A	725	G	O3'-P-O5'	-6.35	94.47	104.00
1	A	1329	A	O3'-P-O5'	-6.35	94.48	104.00
25	a	239	C	O3'-P-O5'	-6.33	94.50	104.00
25	a	1288	G	O3'-P-O5'	-6.33	94.50	104.00
25	a	1238	G	O3'-P-O5'	-6.33	94.51	104.00
1	A	773	G	O3'-P-O5'	-6.31	94.54	104.00
25	a	117	G	C1'-C2'-O2'	6.31	117.86	108.40
25	a	674	G	C1'-C2'-O2'	6.30	117.85	108.40
1	A	332	G	O3'-P-O5'	-6.30	94.55	104.00
25	a	374	A	C2'-C3'-O3'	-6.29	104.27	113.70
25	a	2496	C	O3'-P-O5'	-6.27	94.59	104.00
25	a	1257	C	O3'-P-O5'	-6.27	94.59	104.00
25	a	2094	A	O3'-P-O5'	-6.26	94.60	104.00
26	b	91	C	O3'-P-O5'	-6.26	94.61	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	448	U	O3'-P-O5'	-6.25	94.63	104.00
1	A	645	G	O3'-P-O5'	-6.24	94.64	104.00
1	A	653	U	C1'-C2'-O2'	-6.24	102.44	111.80
25	a	748	G	C1'-O4'-C4'	-6.23	103.67	109.90
25	a	1224	U	O3'-P-O5'	-6.22	94.67	104.00
25	a	470	A	O3'-P-O5'	-6.20	94.71	104.00
25	a	1787	A	C2'-C3'-O3'	-6.20	104.41	113.70
25	a	458	G	O3'-P-O5'	-6.19	94.72	104.00
25	a	1906	G	O3'-P-O5'	-6.18	94.72	104.00
25	a	781	A	C4'-C3'-O3'	-6.14	103.79	113.00
25	a	107	G	C1'-C2'-O2'	6.13	117.60	108.40
1	A	373	A	O3'-P-O5'	-6.12	94.81	104.00
25	a	816	C	O3'-P-O5'	-6.12	94.81	104.00
25	a	1469	A	C1'-C2'-O2'	6.12	117.58	108.40
1	A	113	G	O3'-P-O5'	-6.11	94.83	104.00
1	A	780	A	O3'-P-O5'	-6.11	94.83	104.00
25	a	117	G	C2'-C3'-O3'	-6.10	104.56	113.70
25	a	941	A	O3'-P-O5'	-6.09	94.87	104.00
1	A	570	G	C4'-C3'-O3'	-6.09	103.87	113.00
1	A	1269	A	O3'-P-O5'	-6.08	94.89	104.00
1	A	1222	G	C3'-C2'-O2'	6.07	119.81	110.70
25	a	983	A	C2'-C3'-O3'	-6.07	104.59	113.70
26	b	8	C	O3'-P-O5'	-6.07	94.90	104.00
25	a	1969	A	O3'-P-O5'	-6.06	94.90	104.00
1	A	1522	U	O3'-P-O5'	-6.04	94.94	104.00
25	a	1664	A	O3'-P-O5'	-6.04	94.94	104.00
25	a	2012	G	O3'-P-O5'	-6.02	94.97	104.00
25	a	957	C	O3'-P-O5'	6.01	113.02	104.00
25	a	2600	A	O3'-P-O5'	-6.01	94.99	104.00
1	A	1504	G	O3'-P-O5'	-6.00	95.00	104.00
25	a	2020	A	O3'-P-O5'	-6.00	95.00	104.00
25	a	2491	U	C2'-C3'-O3'	5.99	118.48	109.50
25	a	2826	A	C1'-C2'-O2'	5.98	117.37	108.40
25	a	124	G	O3'-P-O5'	-5.98	95.03	104.00
25	a	705	A	O3'-P-O5'	-5.97	95.04	104.00
25	a	2516	A	O3'-P-O5'	-5.97	95.04	104.00
25	a	1349	C	O3'-P-O5'	-5.97	95.04	104.00
25	a	1847	A	O3'-P-O5'	-5.96	95.06	104.00
25	a	1834	U	C4'-C3'-O3'	-5.94	104.08	113.00
25	a	1516	G	C3'-C2'-O2'	5.93	119.60	110.70
26	b	49	C	O3'-P-O5'	-5.93	95.11	104.00
1	A	960	U	C2'-C3'-O3'	5.92	118.39	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	2847	U	C2'-C3'-O3'	-5.91	104.83	113.70
25	a	2709	G	O3'-P-O5'	-5.88	95.17	104.00
25	a	2242	G	O3'-P-O5'	-5.88	95.18	104.00
25	a	1215	G	C1'-C2'-O2'	5.88	117.22	108.40
25	a	655	A	O3'-P-O5'	-5.87	95.19	104.00
25	a	1298	C	C1'-C2'-O2'	-5.87	99.60	108.40
25	a	1462	C	O3'-P-O5'	-5.86	95.21	104.00
1	A	8	A	O3'-P-O5'	-5.86	95.21	104.00
25	a	856	G	O3'-P-O5'	-5.85	95.22	104.00
25	a	2245	U	C4'-C3'-O3'	-5.85	104.22	113.00
1	A	1431	A	C2'-C3'-O3'	-5.85	104.93	113.70
25	a	245	G	O3'-P-O5'	-5.84	95.23	104.00
25	a	2330	G	O3'-P-O5'	-5.84	95.23	104.00
25	a	198	C	C2'-C3'-O3'	-5.84	104.94	113.70
25	a	1309	G	C1'-C2'-O2'	5.84	117.16	108.40
1	A	1053	G	O3'-P-O5'	-5.83	95.25	104.00
1	A	1512	U	C1'-C2'-O2'	-5.83	99.65	108.40
25	a	255	A	O3'-P-O5'	-5.83	95.26	104.00
25	a	1994	C	C2'-C3'-O3'	-5.82	104.97	113.70
1	A	349	A	O3'-P-O5'	-5.79	95.32	104.00
25	a	1656	C	O3'-P-O5'	-5.78	95.34	104.00
40	p	91	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	563	A	C4'-C3'-O3'	-5.77	104.35	113.00
25	a	528	A	O3'-P-O5'	-5.77	95.34	104.00
1	A	1079	G	O3'-P-O5'	-5.76	95.36	104.00
25	a	1154	G	C2'-C3'-O3'	-5.76	105.06	113.70
1	A	1312	G	O3'-P-O5'	-5.75	95.38	104.00
25	a	452	G	O3'-P-O5'	-5.72	95.42	104.00
25	a	675	A	O3'-P-O5'	-5.71	95.43	104.00
25	a	1378	A	O3'-P-O5'	-5.71	95.43	104.00
25	a	220	G	C2'-C3'-O3'	-5.71	105.13	113.70
25	a	585	G	O3'-P-O5'	-5.70	95.45	104.00
25	a	997	G	C4'-C3'-C2'	-5.70	96.90	102.60
25	a	468	G	O3'-P-O5'	-5.70	95.46	104.00
1	A	965	U	C4'-C3'-O3'	-5.69	104.46	113.00
25	a	792	A	O3'-P-O5'	-5.69	95.47	104.00
25	a	1025	G	C2'-C3'-O3'	5.69	118.04	109.50
25	a	1135	C	C2'-C3'-O3'	5.69	122.23	113.70
25	a	1564	C	O3'-P-O5'	-5.67	95.49	104.00
25	a	1743	G	O3'-P-O5'	-5.67	95.50	104.00
25	a	2634	A	O3'-P-O5'	-5.67	95.50	104.00
25	a	1705	A	O3'-P-O5'	-5.67	95.50	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	120	U	C2'-C3'-O3'	5.66	118.00	109.50
1	A	965	U	C1'-C2'-O2'	-5.66	99.92	108.40
25	a	960	A	C4'-C3'-O3'	-5.66	104.52	113.00
25	a	1570	A	O3'-P-O5'	-5.66	95.52	104.00
1	A	1507	A	O3'-P-O5'	-5.65	95.53	104.00
25	a	860	U	O3'-P-O5'	-5.64	95.53	104.00
1	A	406	G	C2'-C3'-O3'	5.64	122.17	113.70
25	a	940	G	C4'-C3'-C2'	-5.63	96.97	102.60
25	a	2719	G	O3'-P-O5'	-5.63	95.55	104.00
25	a	2824	C	C4'-C3'-O3'	-5.63	104.55	113.00
1	A	5	U	C2'-C3'-O3'	-5.63	105.25	113.70
25	a	784	G	O3'-P-O5'	-5.63	95.56	104.00
25	a	1606	C	O3'-P-O5'	-5.63	95.56	104.00
25	a	573	U	O3'-P-O5'	-5.61	95.58	104.00
12	L	122	PRO	CA-C-O	-5.60	115.23	121.23
25	a	1466	U	O3'-P-O5'	-5.60	95.60	104.00
25	a	1305	C	O3'-P-O5'	-5.60	95.60	104.00
25	a	1774	C	O3'-P-O5'	-5.60	95.60	104.00
25	a	1454	C	O3'-P-O5'	-5.60	95.60	104.00
25	a	1599	U	O3'-P-O5'	-5.59	95.61	104.00
25	a	2844	G	C1'-C2'-O2'	5.59	116.78	108.40
25	a	631	A	C2'-C3'-O3'	-5.58	105.33	113.70
1	A	652	U	O3'-P-O5'	-5.57	95.64	104.00
25	a	2585	U	C4'-C3'-C2'	-5.57	97.03	102.60
1	A	806	C	O3'-P-O5'	-5.55	95.67	104.00
25	a	2870	C	O3'-P-O5'	-5.55	95.67	104.00
1	A	1398	A	O3'-P-O5'	-5.54	95.69	104.00
25	a	577	G	O3'-P-O5'	-5.54	95.69	104.00
1	A	1359	C	O3'-P-O5'	-5.54	95.70	104.00
1	A	1520	C	C2'-C3'-O3'	-5.53	105.41	113.70
1	A	569	C	C2'-C3'-O3'	-5.53	105.41	113.70
25	a	2000	C	O3'-P-O5'	-5.51	95.73	104.00
25	a	703	U	C1'-C2'-O2'	-5.51	100.14	108.40
25	a	681	G	O3'-P-O5'	-5.50	95.75	104.00
25	a	1694	C	O3'-P-O5'	-5.50	95.76	104.00
25	a	1432	G	O3'-P-O5'	-5.49	95.76	104.00
25	a	445	C	O3'-P-O5'	-5.49	95.77	104.00
25	a	2258	C	O3'-P-O5'	-5.49	95.77	104.00
28	d	127	PHE	CA-CB-CG	5.48	119.28	113.80
25	a	716	A	C1'-C2'-O2'	5.48	116.62	108.40
1	A	1302	C	O3'-P-O5'	-5.47	95.79	104.00
25	a	2601	C	O3'-P-O5'	-5.47	95.80	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	2546	U	O3'-P-O5'	-5.47	95.80	104.00
1	A	715	A	C2'-C3'-O3'	-5.46	105.51	113.70
25	a	397	U	O3'-P-O5'	-5.45	95.82	104.00
25	a	111	A	O3'-P-O5'	-5.45	95.83	104.00
25	a	1679	A	O3'-P-O5'	-5.45	95.83	104.00
25	a	763	G	O3'-P-O5'	-5.44	95.83	104.00
1	A	883	C	C1'-C2'-O2'	-5.44	100.24	108.40
1	A	957	U	O3'-P-O5'	-5.44	95.84	104.00
1	A	960	U	C3'-C2'-C1'	-5.44	96.06	101.50
25	a	1525	A	O3'-P-O5'	-5.44	95.84	104.00
25	a	2540	C	O3'-P-O5'	-5.44	95.84	104.00
40	p	31	VAL	N-CA-CB	-5.44	104.61	111.46
25	a	453	A	C2'-C3'-O3'	-5.44	105.55	113.70
1	A	1230	C	C2'-C3'-O3'	-5.43	105.56	113.70
25	a	1866	A	O3'-P-O5'	-5.43	95.86	104.00
25	a	2690	U	O3'-P-O5'	-5.42	95.88	104.00
1	A	803	G	O3'-P-O5'	-5.41	95.88	104.00
1	A	965	U	C3'-C2'-O2'	5.41	118.82	110.70
1	A	1202	U	O3'-P-O5'	-5.40	95.89	104.00
25	a	1905	C	O3'-P-O5'	-5.40	95.90	104.00
25	a	219	A	O3'-P-O5'	-5.40	95.91	104.00
25	a	621	A	O3'-P-O5'	-5.40	95.91	104.00
22	Z	70	G	O3'-P-O5'	-5.39	95.92	104.00
25	a	1138	G	O3'-P-O5'	-5.39	95.92	104.00
25	a	2267	A	O3'-P-O5'	-5.39	95.92	104.00
1	A	794	A	O3'-P-O5'	-5.38	95.93	104.00
26	b	79	G	O3'-P-O5'	-5.38	95.93	104.00
1	A	1250	A	O3'-P-O5'	-5.38	95.94	104.00
1	A	975	A	O3'-P-O5'	-5.37	95.95	104.00
1	A	766	A	O3'-P-O5'	-5.37	95.95	104.00
25	a	1278	C	C1'-C2'-O2'	-5.36	100.36	108.40
25	a	2859	G	O3'-P-O5'	-5.36	95.96	104.00
25	a	2484	G	C4'-C3'-C2'	-5.36	97.24	102.60
1	A	1337	G	O3'-P-O5'	-5.36	95.96	104.00
25	a	2344	U	C2'-C3'-O3'	5.36	117.53	109.50
26	b	14	U	C1'-C2'-O2'	-5.35	103.77	111.80
25	a	1612	C	C4'-C3'-O3'	-5.35	104.97	113.00
1	A	1235	U	O3'-P-O5'	-5.35	95.98	104.00
25	a	623	C	O3'-P-O5'	-5.35	95.98	104.00
1	A	1248	A	O3'-P-O5'	-5.34	95.99	104.00
25	a	689	A	C4'-C3'-C2'	-5.34	97.26	102.60
25	a	2637	U	C2'-C3'-O3'	-5.34	105.69	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	189	G	O3'-P-O5'	-5.34	95.99	104.00
25	a	1857	G	O3'-P-O5'	-5.34	96.00	104.00
1	A	352	C	O3'-P-O5'	-5.33	96.00	104.00
1	A	572	A	O3'-P-O5'	-5.32	96.02	104.00
25	a	2370	G	C4'-C3'-C2'	-5.31	97.29	102.60
25	a	1691	C	C2'-C3'-O3'	-5.31	105.73	113.70
25	a	1255	U	C4'-C3'-O3'	-5.31	105.04	113.00
25	a	2017	U	C2'-C3'-O3'	-5.31	105.73	113.70
25	a	782	A	C2'-C3'-O3'	-5.30	101.54	109.50
25	a	1553	A	O3'-P-O5'	-5.30	96.04	104.00
25	a	2772	C	O3'-P-O5'	-5.30	96.06	104.00
5	E	164	ILE	CA-C-N	-5.29	112.18	121.70
5	E	164	ILE	C-N-CA	-5.29	112.18	121.70
25	a	2837	A	C3'-C2'-O2'	5.29	118.64	110.70
25	a	2687	U	O3'-P-O5'	-5.29	96.07	104.00
25	a	856	G	C1'-C2'-O2'	5.28	116.31	108.40
25	a	1469	A	O3'-P-O5'	-5.27	96.09	104.00
25	a	27	G	C3'-C2'-O2'	-5.26	106.70	114.60
25	a	1337	G	C1'-C2'-O2'	5.26	116.30	108.40
25	a	2585	U	C4'-C3'-O3'	-5.26	105.11	113.00
25	a	465	G	O3'-P-O5'	-5.25	96.12	104.00
25	a	2817	U	C3'-C2'-O2'	5.25	118.58	110.70
25	a	762	U	P-O5'-C5'	-5.25	113.03	120.90
25	a	960	A	C1'-C2'-O2'	5.25	116.27	108.40
25	a	1656	C	C3'-C2'-O2'	5.25	118.57	110.70
1	A	960	U	C3'-C2'-O2'	5.24	122.47	114.60
1	A	790	A	O3'-P-O5'	-5.24	96.14	104.00
25	a	924	G	O3'-P-O5'	-5.24	96.14	104.00
25	a	982	C	O3'-P-O5'	-5.24	96.14	104.00
25	a	1754	A	C2'-C3'-O3'	-5.24	105.84	113.70
25	a	1830	C	C2'-C3'-O3'	-5.23	105.85	113.70
25	a	916	G	O3'-P-O5'	-5.23	96.15	104.00
25	a	827	U	C3'-C2'-O2'	5.23	118.55	110.70
25	a	2427	C	C4'-C3'-O3'	-5.23	105.16	113.00
25	a	1121	C	O3'-P-O5'	-5.21	96.18	104.00
25	a	2375	G	C1'-C2'-O2'	5.21	116.22	108.40
25	a	188	G	C1'-C2'-O2'	5.21	116.21	108.40
25	a	706	A	C3'-C2'-O2'	5.21	118.51	110.70
25	a	2365	G	O3'-P-O5'	-5.21	96.19	104.00
1	A	572	A	C4'-C3'-O3'	-5.21	105.19	113.00
25	a	2272	U	O3'-P-O5'	-5.21	96.19	104.00
25	a	952	G	C4'-C3'-C2'	-5.20	97.40	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	899	C	O3'-P-O5'	-5.20	96.20	104.00
1	A	158	G	O3'-P-O5'	-5.20	96.21	104.00
25	a	953	G	C1'-C2'-O2'	5.20	116.19	108.40
25	a	2467	C	O3'-P-O5'	-5.19	96.21	104.00
1	A	579	A	O3'-P-O5'	-5.19	96.22	104.00
2	B	116	ASP	N-CA-C	-5.18	106.80	113.23
25	a	1249	U	O3'-P-O5'	-5.18	96.23	104.00
25	a	2683	C	O3'-P-O5'	-5.17	96.25	104.00
11	K	36	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	108	G	C4'-C3'-C2'	-5.16	97.44	102.60
25	a	1652	A	C2'-C3'-O3'	-5.16	105.97	113.70
25	a	1678	A	O3'-P-O5'	-5.15	96.27	104.00
1	A	698	G	O3'-P-O5'	-5.14	96.28	104.00
1	A	1236	A	O3'-P-O5'	-5.14	96.28	104.00
25	a	429	A	O3'-P-O5'	-5.14	96.28	104.00
25	a	2502	G	O5'-C5'-C4'	-5.14	103.79	111.50
25	a	2620	C	O3'-P-O5'	-5.14	96.29	104.00
25	a	1888	G	C1'-C2'-O2'	5.14	116.11	108.40
25	a	1993	U	C2'-C3'-O3'	-5.13	106.00	113.70
25	a	2355	G	O3'-P-O5'	-5.13	96.30	104.00
37	m	1	MET	CG-SD-CE	-5.13	89.61	100.90
52	l	14	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	A	1222	G	O3'-P-O5'	-5.12	96.31	104.00
25	a	2629	U	O3'-P-O5'	-5.12	96.32	104.00
25	a	962	G	C2'-C3'-O3'	-5.12	106.02	113.70
25	a	193	U	O3'-P-O5'	-5.11	96.33	104.00
25	a	2268	A	C4'-C3'-C2'	-5.11	97.49	102.60
1	A	294	U	O3'-P-O5'	-5.11	96.34	104.00
50	z	5	GLN	CB-CA-C	-5.11	100.77	109.65
1	A	1231	G	O3'-P-O5'	-5.09	96.36	104.00
27	c	39	LYS	N-CA-CB	-5.09	102.31	110.46
25	a	685	A	C4'-C3'-O3'	5.09	117.03	109.40
25	a	2053	G	C4'-C3'-C2'	-5.08	97.52	102.60
25	a	2329	U	P-O5'-C5'	-5.08	113.27	120.90
23	X	21	C	O3'-P-O5'	-5.08	96.38	104.00
25	a	2354	C	C4'-C3'-C2'	-5.08	97.52	102.60
1	A	410	G	C2'-C3'-O3'	-5.08	106.08	113.70
25	a	1470	A	C2'-C3'-O3'	-5.08	106.08	113.70
25	a	1785	A	O3'-P-O5'	-5.07	96.39	104.00
25	a	1279	G	C4'-C3'-C2'	-5.07	97.53	102.60
1	A	1065	U	O3'-P-O5'	-5.06	96.40	104.00
1	A	1316	G	C1'-C2'-O2'	5.06	115.99	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	846	U	C2'-C3'-O3'	-5.06	106.11	113.70
25	a	1148	U	C4'-C3'-C2'	-5.06	97.54	102.60
25	a	2050	C	C4'-C3'-O3'	-5.06	105.41	113.00
25	a	457	A	C1'-C2'-O2'	5.06	119.39	111.80
25	a	855	G	O3'-P-O5'	-5.05	96.42	104.00
25	a	527	C	O3'-P-O5'	-5.05	96.42	104.00
25	a	2761	A	O3'-P-O5'	-5.05	96.42	104.00
25	a	2550	G	C4'-C3'-O3'	-5.05	105.43	113.00
25	a	1252	G	C4'-C3'-O3'	-5.04	101.83	109.40
25	a	2526	G	C4'-C3'-C2'	-5.04	97.56	102.60
25	a	570	G	P-O3'-C3'	5.04	127.76	120.20
25	a	1293	C	O3'-P-O5'	-5.04	96.44	104.00
25	a	192	C	C2'-C3'-O3'	-5.03	106.15	113.70
25	a	1569	A	O3'-P-O5'	-5.03	96.45	104.00
1	A	1392	G	C4'-C3'-C2'	-5.03	97.57	102.60
25	a	802	A	C4'-C3'-O3'	-5.03	105.45	113.00
25	a	2238	G	C2'-C3'-O3'	5.03	117.04	109.50
1	A	819	A	C2'-C3'-O3'	5.02	117.03	109.50
25	a	1358	G	O3'-P-O5'	-5.02	96.47	104.00
25	a	378	C	C4'-C3'-C2'	-5.01	97.58	102.60
25	a	691	C	O3'-P-O5'	-5.01	96.48	104.00
25	a	476	G	O3'-P-O5'	-5.01	96.49	104.00
1	A	305	G	C2'-C3'-O3'	5.01	117.01	109.50
1	A	688	G	O3'-P-O5'	-5.01	96.49	104.00
1	A	108	G	O4'-C1'-C2'	-5.00	102.59	107.60
25	a	1905	C	C4'-C3'-O3'	-5.00	105.49	113.00
25	a	2051	A	O3'-P-O5'	-5.00	96.50	104.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	1	41	ARG	Sidechain
53	2	13	ARG	Sidechain
54	3	36	ARG	Sidechain
4	D	63	ARG	Sidechain
8	H	117	ARG	Sidechain
9	I	41	ARG	Sidechain
10	J	62	ARG	Sidechain
10	J	7	ARG	Sidechain
13	M	107	ARG	Sidechain
14	N	85	ARG	Sidechain

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Mol	Chain	Res	Type	Group
33	i	120	ARG	Sidechain
40	p	13	ARG	Sidechain
40	p	51	ARG	Sidechain
41	q	84	ARG	Sidechain
43	s	69	ARG	Sidechain
46	v	14	ARG	Sidechain
48	x	29	ARG	Sidechain

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	32825	0	16539	161	0
2	B	1753	0	1780	24	0
3	C	1624	0	1696	2	0
4	D	1643	0	1707	20	0
5	E	1152	0	1196	2	0
6	F	839	0	833	1	0
7	G	1203	0	1254	6	0
8	H	979	0	1031	1	0
9	I	1022	0	1070	4	0
10	J	786	0	828	5	0
11	K	877	0	884	2	0
12	L	957	0	1017	2	0
13	M	891	0	952	10	0
14	N	805	0	844	2	0
15	O	714	0	734	1	0
16	P	643	0	661	3	0
17	Q	641	0	682	5	0
18	R	544	0	565	2	0
19	S	668	0	693	5	0
20	T	670	0	719	1	0
21	U	589	0	629	3	0
22	V	1623	0	825	27	0
22	Z	1623	0	825	18	0
23	X	240	0	121	0	0
24	Y	2000	0	1020	19	0
25	a	59130	0	29768	181	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	b	2549	0	1291	14	0
27	c	2082	0	2154	5	0
28	d	1566	0	1618	1	0
29	e	1552	0	1619	1	0
30	f	1410	0	1444	25	0
31	g	1295	0	1332	0	0
32	h	303	0	327	0	0
33	i	1129	0	1162	2	0
34	j	946	0	1023	11	0
35	k	1053	0	1129	3	0
36	l	1075	0	1145	5	0
37	m	945	0	989	0	0
38	n	892	0	923	9	0
39	o	917	0	962	3	0
40	p	947	0	1019	3	0
41	q	816	0	839	3	0
42	r	857	0	922	3	0
43	s	738	0	807	1	0
44	t	779	0	831	4	0
45	u	753	0	780	1	0
46	v	628	0	642	2	0
47	w	625	0	652	2	0
48	x	495	0	526	1	0
49	y	449	0	488	1	0
50	z	444	0	458	2	0
51	0	417	0	451	0	0
52	1	377	0	418	2	0
53	2	504	0	572	1	0
54	3	302	0	340	2	0
55	4	480	0	478	12	0
56	A	93	0	0	0	0
56	Y	6	0	0	0	0
56	a	206	0	0	0	0
56	b	5	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
56	m	1	0	0	0	0
56	z	1	0	0	0	0
57	a	60	0	114	2	0
58	a	14	0	26	1	0
59	a	36	0	72	0	0
60	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	4	1	0	0	0	0
All	All	144192	0	96426	547	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 2.

All (547) 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)
2:B:4:VAL:HG11	2:B:50:PHE:HD2	1.36	0.90
22:V:37:A:H3'	22:V:38:A:H8	1.37	0.89
2:B:119:THR:O	2:B:123:ASP:HB2	1.73	0.88
4:D:105:MET:HE1	4:D:180:GLY:HA3	1.56	0.85
1:A:429:U:H3'	4:D:9:LEU:HD12	1.59	0.83
2:B:4:VAL:HG11	2:B:50:PHE:CD2	2.14	0.81
30:f:158:THR:HG22	30:f:160:ALA:H	1.47	0.79
1:A:1457:G:H2'	1:A:1458:G:H5''	1.65	0.76
1:A:1100:C:H3'	2:B:95:ARG:HH12	1.50	0.75
4:D:155:VAL:HG11	4:D:178:MET:HE1	1.69	0.74
1:A:83:C:H2'	1:A:86:G:H1	1.50	0.74
1:A:437:U:H5''	1:A:437:U:H6	1.53	0.74
1:A:664:G:H22	1:A:741:G:H1	1.36	0.73
1:A:1027:C:H2'	1:A:1028:C:H6	1.52	0.73
22:V:37:A:H3'	22:V:38:A:C8	2.23	0.71
22:V:18:G:H21	22:V:58:A:H5'	1.56	0.71
1:A:74:A:H2'	1:A:75:G:C8	2.26	0.70
22:Z:62:C:H2'	22:Z:63:G:C8	2.27	0.70
25:a:1047:G:HO2'	25:a:1110:G:H1	0.72	0.70
13:M:79:ARG:NH2	55:4:56:ARG:NE	2.42	0.68
1:A:345:C:OP2	39:o:37:LYS:NZ	2.25	0.68
1:A:411:A:H4'	1:A:412:A:O5'	1.95	0.67
1:A:1423:G:H5'	34:j:49:ARG:HH22	1.59	0.67
25:a:1115:G:O2'	25:a:1116:G:O5'	2.09	0.66
1:A:1356:G:H2'	1:A:1357:A:C8	2.30	0.66
26:b:36:C:N4	26:b:49:C:O2	2.28	0.66
25:a:2585:U:O2'	25:a:2586:U:H5'	1.95	0.66
1:A:1027:C:H2'	1:A:1028:C:C6	2.31	0.65
1:A:1396:A:H4'	1:A:1397:C:H5''	1.77	0.65
22:Z:21:A:H61	22:Z:46:G:H2'	1.60	0.65
1:A:1124:G:OP1	10:J:37:ARG:NH1	2.29	0.65
25:a:958:U:H2'	26:b:89:U:O2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:A:H2'	1:A:947:G:C8	2.31	0.65
1:A:1:A:C6	1:A:2:A:C6	2.84	0.65
4:D:105:MET:HE3	4:D:173:VAL:HG13	1.80	0.64
1:A:458:U:H3	1:A:474:G:H1	1.44	0.64
4:D:114:ALA:O	4:D:118:VAL:HG23	1.98	0.64
25:a:1778:U:H2'	25:a:1784:A:N6	2.13	0.64
1:A:208:U:H3	1:A:211:G:H1	1.44	0.64
13:M:8:ASN:ND2	30:f:143:TYR:CE1	2.67	0.63
42:r:4:ILE:HG22	42:r:106:VAL:HG22	1.81	0.62
13:M:79:ARG:NH2	55:4:56:ARG:CZ	2.62	0.62
22:V:35:A:H2'	22:V:37:A:C8	2.35	0.62
1:A:339:C:C5	34:j:98:ARG:NH1	2.68	0.62
1:A:1100:C:H3'	2:B:95:ARG:NH1	2.14	0.62
1:A:677:U:H3	1:A:713:G:H22	1.45	0.62
22:Z:62:C:H2'	22:Z:63:G:H8	1.63	0.61
30:f:105:THR:HA	55:4:38:SER:HB2	1.81	0.61
25:a:2014:A:H2'	25:a:2015:A:C8	2.36	0.61
4:D:124:MET:HE3	4:D:146:ARG:HG2	1.83	0.61
30:f:37:ASN:HB3	30:f:153:ASP:OD1	2.01	0.61
25:a:784:G:H5'	25:a:785:G:OP1	2.01	0.60
24:Y:47(A):C:H2'	24:Y:47(B):G:H8	1.66	0.60
26:b:48:U:O2'	38:n:100:HIS:HE1	1.83	0.60
1:A:80:A:H3'	1:A:81:A:H8	1.66	0.60
25:a:1870:C:O2'	25:a:1871:A:O4'	2.20	0.60
6:F:99:ALA:HB1	6:F:103:VAL:HG23	1.82	0.60
22:Z:5:G:H1	22:Z:68:C:H42	1.49	0.60
25:a:2505:G:HO2'	25:a:2506:U:H6	1.49	0.60
1:A:1:A:N6	1:A:2:A:C6	2.70	0.60
22:Z:66:C:H2'	22:Z:67:C:C6	2.37	0.60
25:a:49:A:H5''	25:a:51:G:O4'	2.02	0.60
22:V:65:C:H2'	22:V:66:C:C6	2.36	0.59
22:Z:43:A:H2'	22:Z:44:A:C8	2.37	0.59
25:a:881:G:H1	25:a:895:U:H3	1.48	0.59
19:S:9:PRO:HD3	55:4:64:PHE:CD1	2.37	0.59
7:G:76:LYS:HE3	7:G:89:VAL:HG21	1.84	0.59
25:a:299:A:N3	25:a:319:G:O2'	2.35	0.59
1:A:1101:A:OP2	2:B:95:ARG:NH1	2.36	0.58
25:a:933:A:H5'	25:a:934:U:OP2	2.02	0.58
1:A:95:C:H2'	1:A:96:U:C6	2.39	0.58
2:B:4:VAL:CG1	2:B:50:PHE:HD2	2.13	0.58
22:V:21:A:H61	22:V:46:G:H2'	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:1607:C:N4	25:a:1622:G:OP2	2.22	0.58
1:A:151:A:OP2	1:A:169:C:N4	2.37	0.58
2:B:76:ALA:O	2:B:80:VAL:HG23	2.03	0.58
25:a:69:C:O2'	25:a:70:G:H5'	2.04	0.58
4:D:101:VAL:O	4:D:105:MET:HG2	2.03	0.57
25:a:568:U:H1'	25:a:2030:6MZ:H9C1	1.86	0.57
1:A:71:A:N1	1:A:99:C:O2'	2.36	0.57
25:a:1141:U:H4'	25:a:1142:A:O4'	2.04	0.57
25:a:221:A:N1	25:a:265:A:O2'	2.37	0.57
25:a:1980:G:O2'	25:a:1982:U:OP2	2.22	0.57
22:V:11:A:H2'	22:V:12:G:O4'	2.04	0.57
1:A:1003:G:N2	1:A:1004:A:O2'	2.38	0.56
7:G:2:PRO:HD3	7:G:7:ILE:HD11	1.87	0.56
25:a:2312:U:H5'	30:f:85:ILE:HD11	1.86	0.56
1:A:109:A:H2'	1:A:326:G:N2	2.21	0.56
25:a:1296:G:OP1	25:a:2709:G:O2'	2.23	0.56
4:D:155:VAL:CG1	4:D:178:MET:HE1	2.35	0.56
22:Z:21:A:N6	22:Z:46:G:H2'	2.20	0.56
25:a:1509:A:HO2'	25:a:1510:G:H8	1.53	0.56
24:Y:37:T6A:N1	24:Y:37:T6A:N11	2.51	0.56
25:a:634:C:H2'	25:a:635:C:C6	2.41	0.56
2:B:80:VAL:HG22	2:B:214:LEU:HD11	1.86	0.56
24:Y:8:4SU:H5''	24:Y:49:C:OP2	2.05	0.56
25:a:1027:A:C2	25:a:2488:G:H5'	2.41	0.55
1:A:1086:U:H3	1:A:1099:G:H22	1.55	0.55
26:b:45:A:C4	26:b:46:A:C8	2.95	0.55
1:A:999:C:N3	1:A:1042:A:N6	2.55	0.55
25:a:2327:A:H2'	25:a:2328:A:C8	2.41	0.55
25:a:2430:A:N3	25:a:2430:A:H2'	2.21	0.55
44:t:50:PRO:HA	44:t:54:GLN:HB3	1.89	0.55
1:A:429:U:H3'	4:D:9:LEU:CD1	2.33	0.54
1:A:1025:U:H4'	1:A:1026:G:H8	1.71	0.54
36:l:66:ARG:NH1	36:l:104:GLU:OE2	2.40	0.54
4:D:104:ARG:HB3	4:D:168:PRO:HG2	1.88	0.54
22:Z:66:C:H2'	22:Z:67:C:H6	1.71	0.54
16:P:6:LEU:CD2	16:P:19:VAL:HG22	2.38	0.54
1:A:339:C:H5	34:j:98:ARG:HH12	1.54	0.54
22:Z:18:G:H21	22:Z:58:A:H5'	1.73	0.54
25:a:2273:A:H2'	25:a:2274:A:C8	2.42	0.54
25:a:1607:C:H4'	25:a:1608:A:O5'	2.08	0.54
30:f:140:GLU:OE2	55:4:26:SER:OG	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:U:H3'	1:A:1009:U:H5''	1.90	0.54
2:B:4:VAL:CG1	2:B:9:MET:HE3	2.37	0.54
25:a:588:U:H2'	25:a:589:U:C6	2.43	0.54
25:a:875:G:C6	25:a:876:C:C4	2.96	0.54
25:a:1682:G:C8	25:a:1757:A:C2	2.96	0.53
25:a:1021:A:H3'	25:a:1021:A:N3	2.23	0.53
25:a:285:G:C6	25:a:356:G:C6	2.97	0.53
25:a:2343:U:HO2'	25:a:2373:G:HO2'	1.57	0.53
13:M:67:GLY:HA3	30:f:113:ASP:CG	2.34	0.53
25:a:1386:C:H2'	25:a:1387:A:C8	2.44	0.53
54:3:16:ILE:HD13	54:3:25:VAL:HG22	1.91	0.53
25:a:277:G:H4'	25:a:278:A:O5'	2.09	0.52
25:a:549:G:H2'	25:a:550:C:C6	2.45	0.52
1:A:539:A:H2'	1:A:540:G:C8	2.45	0.52
2:B:66:LYS:NZ	2:B:157:LEU:O	2.37	0.52
27:c:29:PRO:HG2	27:c:34:LEU:HD11	1.90	0.52
30:f:112:ARG:HH12	30:f:133:ARG:HH22	1.57	0.52
1:A:8:A:N6	4:D:202:GLU:O	2.43	0.52
24:Y:47(N):C:H2'	24:Y:47(O):A:C8	2.45	0.52
1:A:1347:G:O6	9:I:12:ARG:NH2	2.37	0.52
25:a:2328:A:H2'	25:a:2329:U:C6	2.44	0.52
24:Y:47(I):A:C4	24:Y:47(J):G:H1'	2.45	0.52
30:f:142:ASP:HB3	30:f:145:LYS:HB2	1.92	0.52
1:A:339:C:H5	34:j:98:ARG:NH1	2.07	0.51
2:B:154:MET:HG3	2:B:156:GLY:O	2.11	0.51
1:A:1218:C:H2'	1:A:1219:A:C8	2.46	0.51
25:a:1720:U:H2'	25:a:1721:G:O4'	2.11	0.51
22:V:55:U:H2'	22:V:56:C:H2'	1.91	0.51
25:a:1509:A:O2'	25:a:1510:G:H8	1.93	0.51
25:a:1641:A:H2'	25:a:1642:G:O4'	2.09	0.51
1:A:56:U:H2'	1:A:57:G:C8	2.46	0.51
25:a:1299:G:H5''	25:a:1300:G:OP1	2.11	0.51
12:L:7:LEU:HB3	17:Q:34:TYR:CZ	2.46	0.51
2:B:133:GLU:O	2:B:137:ARG:HG3	2.11	0.51
3:C:35:SER:OG	3:C:59:ARG:NH2	2.44	0.51
22:V:61:C:H2'	22:V:62:C:C6	2.45	0.51
25:a:875:G:C5	25:a:876:C:C4	2.99	0.51
1:A:437:U:H2'	1:A:438:U:O4'	2.11	0.51
1:A:1273:C:H2'	1:A:1274:A:O4'	2.11	0.51
25:a:1450:G:C6	25:a:1451:C:N4	2.79	0.51
1:A:147:G:H2'	1:A:148:G:C8	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:A:H2'	1:A:172:A:C8	2.45	0.50
1:A:1456:A:H2'	1:A:1457:G:O4'	2.11	0.50
25:a:2395:C:H2'	25:a:2396:G:O4'	2.10	0.50
30:f:135:GLN:HG2	30:f:141:ILE:HG21	1.94	0.50
25:a:118:A:O5'	25:a:119:A:H5''	2.12	0.50
26:b:42:C:C6	30:f:66:LEU:HB2	2.46	0.50
1:A:371:A:H2'	1:A:372:C:O4'	2.11	0.50
22:Z:67:C:C2'	22:Z:68:C:H5'	2.41	0.50
22:Z:72:A:H2'	22:Z:73:A:O4'	2.11	0.50
1:A:1088:G:H4'	21:U:70:LEU:HD13	1.93	0.50
22:V:20:U:O4	22:V:60:U:N3	2.44	0.50
1:A:714:G:H2'	1:A:715:A:C8	2.46	0.50
22:Z:23:C:H2'	22:Z:24:U:C6	2.47	0.50
1:A:1025:U:H4'	1:A:1026:G:C8	2.47	0.50
24:Y:22:A:H2'	24:Y:23:G:O4'	2.12	0.50
24:Y:47(H):A:H2'	24:Y:47(I):A:C8	2.46	0.50
26:b:66:A:H61	26:b:107:G:H2'	1.76	0.50
1:A:620:C:H2'	1:A:621:A:C8	2.46	0.50
25:a:1047:G:O2'	25:a:1110:G:N1	2.24	0.50
25:a:12:U:H2'	25:a:12:U:O2	2.11	0.49
18:R:10:PHE:HE1	18:R:15:ALA:CB	2.24	0.49
22:V:9:G:H4'	22:V:10:G:OP2	2.12	0.49
25:a:864:G:C6	25:a:865:C:N4	2.81	0.49
19:S:42:PRO:HD3	55:4:60:PHE:CE2	2.48	0.49
25:a:2788:C:H2'	25:a:2789:C:C6	2.48	0.49
1:A:673:A:H2'	1:A:674:G:C8	2.47	0.49
1:A:1228:C:H1'	13:M:116:ILE:HD11	1.94	0.49
1:A:82:G:C5	1:A:83:C:H1'	2.48	0.49
1:A:1326:U:H2'	1:A:1327:C:H6	1.77	0.49
35:k:23:ILE:HG12	41:q:82:HIS:CD2	2.48	0.49
25:a:945:A:H1'	57:a:6207:SPD:H82	1.93	0.49
25:a:1590:A:H2'	25:a:1591:A:H8	1.78	0.49
26:b:1:U:H2'	26:b:2:G:H8	1.78	0.49
33:i:4:PHE:O	40:p:64:ARG:NH2	2.42	0.49
25:a:1020:A:N1	25:a:1141:U:O2'	2.41	0.49
1:A:594:U:H2'	1:A:595:A:O4'	2.13	0.48
25:a:1790:C:O2'	27:c:208:ALA:HB2	2.13	0.48
25:a:1590:A:H2'	25:a:1591:A:C8	2.48	0.48
19:S:65:GLU:HA	55:4:56:ARG:HG3	1.94	0.48
1:A:1023:U:H2'	1:A:1024:G:H8	1.79	0.48
22:V:16:C:H5'	22:V:17:C:C5	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:657:U:H2'	25:a:658:U:C6	2.48	0.48
38:n:2:ASP:N	38:n:2:ASP:OD1	2.47	0.48
1:A:410:G:OP2	4:D:31:LYS:HE2	2.13	0.48
1:A:1009:U:H3	1:A:1020:G:H1	1.59	0.48
22:V:62:C:H2'	22:V:63:G:H8	1.77	0.48
25:a:1544:A:C6	25:a:1545:A:C6	3.02	0.48
57:a:6211:SPD:H72	42:r:87:PRO:O	2.13	0.48
25:a:1434:A:H2'	25:a:1435:G:H8	1.78	0.48
25:a:2236:U:H2'	25:a:2237:G:O4'	2.14	0.48
26:b:66:A:N6	26:b:107:G:H2'	2.28	0.48
34:j:41:ILE:CD1	34:j:86:LEU:HD22	2.44	0.48
7:G:16:PRO:HB2	9:I:42:GLU:HB3	1.96	0.48
25:a:1020:A:C2	25:a:1141:U:C2	3.01	0.48
35:k:57:LEU:HD22	53:2:54:ASP:HB3	1.95	0.48
1:A:1004:A:H2'	1:A:1005:A:O4'	2.14	0.48
22:V:18:G:C8	22:V:18:G:H5'	2.48	0.48
25:a:355:U:H2'	25:a:356:G:H8	1.79	0.48
25:a:984:A:N3	25:a:984:A:H2'	2.28	0.48
30:f:116:GLY:HA3	30:f:178:ARG:HB3	1.96	0.48
2:B:66:LYS:HE3	2:B:157:LEU:O	2.13	0.48
13:M:8:ASN:ND2	30:f:143:TYR:CD1	2.82	0.48
1:A:1068:G:N7	1:A:1094:G:H2'	2.29	0.47
25:a:634:C:H2'	25:a:635:C:H6	1.78	0.47
25:a:1478:G:H1	25:a:1513:U:H3	1.62	0.47
25:a:2680:U:O2'	25:a:2681:C:H5'	2.13	0.47
29:e:153:LEU:HD21	29:e:158:PHE:HB2	1.95	0.47
44:t:53:ASN:ND2	44:t:55:PRO:O	2.47	0.47
1:A:1024:G:H3'	1:A:1025:U:C6	2.49	0.47
14:N:10:GLU:HG3	14:N:63:ARG:HD2	1.96	0.47
22:Z:5:G:H1	22:Z:68:C:N4	2.11	0.47
1:A:216:U:H2'	1:A:217:C:C6	2.49	0.47
1:A:90:C:H2'	1:A:91:U:C6	2.49	0.47
30:f:95:ARG:CZ	55:4:1:MET:HE2	2.45	0.47
2:B:4:VAL:HG13	2:B:9:MET:HE3	1.96	0.47
10:J:66:GLU:HB2	14:N:99:ALA:HB2	1.96	0.47
25:a:1111:A:N3	25:a:1112:G:H1'	2.28	0.47
25:a:276:U:H2'	25:a:277:G:C8	2.50	0.47
25:a:2080:A:H5'	47:w:19:SER:HB2	1.97	0.47
25:a:2547:A:H2'	25:a:2548:U:C6	2.50	0.47
1:A:208:U:H2'	1:A:209:U:O4'	2.13	0.47
1:A:1244:G:C6	1:A:1245:C:C4	3.01	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:1378:A:O2'	25:a:1380:G:N7	2.42	0.47
25:a:2545:G:H2'	25:a:2546:U:O4'	2.14	0.47
48:x:61:ALA:O	48:x:62:GLY:C	2.57	0.47
1:A:1:A:N6	1:A:2:A:N1	2.63	0.47
24:Y:13:G:H5''	24:Y:13:G:H8	1.80	0.47
25:a:930:G:H1'	49:y:25:LEU:HD11	1.97	0.47
25:a:1637:A:H5'	25:a:1760:C:O2'	2.15	0.47
30:f:44:ILE:HA	30:f:83:TYR:CE2	2.49	0.47
34:j:121:GLU:OE1	39:o:65:SER:OG	2.33	0.47
1:A:107:G:N7	20:T:10:ARG:NH2	2.62	0.47
1:A:1014:A:C2	1:A:1219:A:H1'	2.50	0.47
1:A:1530:G:H2'	1:A:1531:A:C8	2.49	0.47
24:Y:47(I):A:C5	24:Y:47(J):G:H1'	2.50	0.47
22:V:31:G:H3'	22:V:32:C:H6	1.80	0.47
1:A:1007:U:H2'	1:A:1008:U:H6	1.80	0.46
7:G:4:ARG:O	7:G:5:ARG:C	2.59	0.46
10:J:85:ASP:HB3	10:J:89:ARG:HH21	1.80	0.46
22:V:65:C:H2'	22:V:66:C:H6	1.80	0.46
25:a:1544:A:N1	25:a:1545:A:C2	2.83	0.46
25:a:900:A:C5	25:a:901:C:C5	3.03	0.46
25:a:1149:G:H2'	25:a:1150:C:C6	2.51	0.46
1:A:1:A:C5	1:A:2:A:C5	3.04	0.46
22:V:32:C:H2'	22:V:33:U:O4'	2.16	0.46
34:j:58:LEU:HD11	34:j:86:LEU:HD13	1.98	0.46
1:A:1326:U:H2'	1:A:1327:C:C6	2.51	0.46
22:V:8:U:H1'	22:V:21:A:H2	1.79	0.46
22:Z:12:G:H5''	25:a:1908:C:O2'	2.16	0.46
22:V:66:C:H2'	22:V:67:C:C6	2.50	0.46
25:a:1761:C:O5'	25:a:1761:C:H6	1.98	0.46
1:A:1:A:C5	1:A:2:A:C6	3.03	0.46
24:Y:47(L):U:H2'	24:Y:47(M):G:H8	1.80	0.46
25:a:55:G:O2'	25:a:127:A:N1	2.45	0.46
25:a:2321:U:H2'	25:a:2321:U:O2	2.15	0.46
25:a:2818:U:HO2'	25:a:2836:U:HO2'	1.64	0.46
4:D:98:LEU:HB2	4:D:135:TYR:HB3	1.98	0.46
17:Q:64:CYS:SG	17:Q:74:THR:HG23	2.55	0.46
25:a:2038:G:H2'	25:a:2039:U:O4'	2.16	0.46
1:A:175:C:H2'	1:A:176:C:H6	1.81	0.46
7:G:151:PHE:CZ	11:K:56:ARG:HG2	2.51	0.46
25:a:1434:A:H2'	25:a:1435:G:C8	2.51	0.46
25:a:1589:U:H2'	25:a:1590:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:2219:U:H2'	25:a:2220:U:O4'	2.15	0.46
25:a:2251:OMG:HM23	25:a:2251:OMG:H1'	1.64	0.46
25:a:1182:G:H2'	25:a:1183:U:O4'	2.16	0.46
25:a:2282:G:H4'	25:a:2389:G:O2'	2.16	0.46
4:D:97:ARG:O	4:D:101:VAL:HG23	2.16	0.45
18:R:10:PHE:CG	18:R:10:PHE:O	2.69	0.45
36:l:80:VAL:HA	46:v:5:LYS:O	2.16	0.45
1:A:337:G:H2'	1:A:338:A:C8	2.51	0.45
13:M:79:ARG:NH2	55:4:56:ARG:CD	2.79	0.45
25:a:1799:G:O2'	27:c:180:GLU:OE2	2.31	0.45
1:A:1004:A:N6	1:A:1026:G:H1'	2.31	0.45
25:a:962:G:O2'	25:a:2496:C:O2'	2.33	0.45
1:A:2:A:H2'	1:A:3:A:C8	2.52	0.45
1:A:1391:U:H2'	1:A:1392:G:C8	2.52	0.45
2:B:66:LYS:CE	2:B:157:LEU:O	2.65	0.45
24:Y:75:C:H2'	24:Y:76:A:C8	2.52	0.45
25:a:876:C:H2'	25:a:877:A:O4'	2.16	0.45
25:a:1009:A:N3	25:a:1153:C:O2'	2.47	0.45
25:a:2020:A:H5'	50:z:9:THR:CG2	2.46	0.45
25:a:2687:U:O5'	25:a:2687:U:H6	1.99	0.45
38:n:39:VAL:HB	38:n:49:VAL:HG22	1.99	0.45
1:A:604:G:H2'	1:A:605:U:O4'	2.17	0.45
4:D:134:SER:O	4:D:135:TYR:C	2.59	0.45
22:V:4:G:O2'	22:V:5:G:H5'	2.17	0.45
25:a:84:A:N1	25:a:98:G:O2'	2.40	0.45
25:a:280:U:H2'	25:a:281:C:C6	2.52	0.45
25:a:479:A:N3	25:a:481:G:H5''	2.31	0.45
25:a:1937:A:H1'	25:a:1939:5MU:H72	1.97	0.45
2:B:4:VAL:HG12	2:B:51:ASN:OD1	2.16	0.45
25:a:57:C:H2'	25:a:58:G:O4'	2.17	0.45
22:V:18:G:N2	22:V:58:A:OP2	2.50	0.45
25:a:295:G:C2	25:a:296:U:C5	3.04	0.45
25:a:395:U:O2'	25:a:396:G:N7	2.48	0.45
25:a:1482:G:N1	25:a:1508:A:H2	2.14	0.45
30:f:22:TYR:OH	30:f:165:GLU:HG2	2.17	0.45
1:A:1287:A:C6	1:A:1288:A:C6	3.05	0.45
25:a:182:A:C6	25:a:183:C:C4	3.05	0.45
25:a:1874:C:H2'	25:a:1875:G:O4'	2.17	0.45
1:A:71:A:H61	1:A:99:C:H1'	1.81	0.45
1:A:205:A:H2'	1:A:206:C:O4'	2.17	0.45
1:A:1031:C:O3'	1:A:1032:G:N2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:278:A:N6	25:a:362:A:N7	2.64	0.45
34:j:41:ILE:HD11	34:j:86:LEU:HD22	1.99	0.45
42:r:20:VAL:HG11	42:r:44:ALA:HA	1.99	0.45
22:V:62:C:H2'	22:V:63:G:C8	2.51	0.45
25:a:2321:U:O2	25:a:2321:U:C2'	2.64	0.45
26:b:24:G:N7	26:b:56:G:H2'	2.32	0.45
1:A:1371:G:O3'	9:I:71:GLY:HA3	2.16	0.44
25:a:1115:G:HO2'	25:a:1116:G:P	2.36	0.44
26:b:28:C:C2	26:b:29:A:C8	3.05	0.44
28:d:62:LYS:N	28:d:63:PRO:HD2	2.33	0.44
1:A:160:A:H2'	1:A:161:A:O4'	2.17	0.44
1:A:545:C:OP1	4:D:58:LYS:NZ	2.50	0.44
1:A:1086:U:O5'	1:A:1086:U:C6	2.70	0.44
30:f:36:LEU:O	30:f:88:LYS:HA	2.17	0.44
1:A:975:A:H8	1:A:1357:A:HO2'	1.63	0.44
24:Y:5:A:H2'	24:Y:6:G:H5''	1.99	0.44
25:a:273:G:C6	25:a:274:C:N4	2.85	0.44
25:a:295:G:C2	25:a:296:U:C6	3.06	0.44
25:a:1656:C:O5'	25:a:1656:C:H6	2.00	0.44
4:D:119:SER:C	4:D:121:LYS:H	2.26	0.44
25:a:1509:A:O2'	25:a:1510:G:C8	2.69	0.44
1:A:994:A:C8	1:A:1216:A:H4'	2.53	0.44
2:B:61:ALA:CB	2:B:221:VAL:HG13	2.47	0.44
8:H:64:LYS:HG3	8:H:71:VAL:HG21	2.00	0.44
22:Z:8:U:H2'	22:Z:46:G:H21	1.82	0.44
25:a:644:A:H2'	25:a:645:C:O4'	2.18	0.44
25:a:811:U:H2'	35:k:21:ARG:HA	1.99	0.44
44:t:54:GLN:HG2	44:t:55:PRO:HD3	1.99	0.44
1:A:451:A:H61	1:A:481:G:H5'	1.83	0.44
1:A:1008:U:H5'	1:A:1009:U:OP2	2.18	0.44
25:a:1263:U:H2'	25:a:1264:A:C8	2.52	0.44
25:a:2494:G:O2'	36:l:79:ALA:HA	2.18	0.44
38:n:56:LYS:HD2	38:n:56:LYS:N	2.32	0.44
55:4:41:HIS:CD2	55:4:43:PHE:H	2.35	0.44
1:A:82:G:N3	1:A:82:G:H2'	2.33	0.44
1:A:986:U:H2'	1:A:987:G:O4'	2.17	0.44
1:A:1278:G:O5'	1:A:1279:G:H5'	2.17	0.44
13:M:79:ARG:HH22	55:4:56:ARG:CZ	2.31	0.44
25:a:1039:A:H2'	25:a:1040:A:O4'	2.18	0.44
1:A:404:G:O2'	1:A:498:A:N1	2.45	0.43
25:a:1589:U:H2'	25:a:1590:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:U:H4'	1:A:86:G:C2	2.53	0.43
1:A:459:A:H2'	1:A:460:A:C8	2.53	0.43
22:V:17:C:OP1	22:V:61:C:H5'	2.19	0.43
22:V:66:C:H2'	22:V:67:C:H6	1.83	0.43
25:a:396:G:OP2	47:w:10:LYS:NZ	2.48	0.43
38:n:53:THR:HG21	38:n:70:ALA:HB1	2.00	0.43
25:a:832:U:H2'	25:a:833:A:C8	2.52	0.43
25:a:1519:G:C5	25:a:1520:U:C4	3.07	0.43
3:C:110:GLU:HB2	3:C:144:LEU:HD12	1.99	0.43
25:a:742:A:H2'	25:a:743:A:C8	2.53	0.43
1:A:131:A:H2'	1:A:132:C:C6	2.53	0.43
1:A:745:G:H2'	1:A:746:A:C8	2.54	0.43
1:A:923:A:O2'	1:A:1399:C:OP2	2.32	0.43
1:A:1496:C:H2'	1:A:1497:G:O4'	2.19	0.43
25:a:570:G:H2'	25:a:2030:6MZ:N7	2.34	0.43
25:a:2845:U:H5''	39:o:52:ASN:O	2.19	0.43
1:A:349:A:O2'	1:A:350:G:H5'	2.18	0.43
1:A:1028:C:O2	1:A:1028:C:H2'	2.18	0.43
1:A:37:U:O2'	1:A:500:G:H4'	2.19	0.43
1:A:1038:C:C2	1:A:1039:G:C8	3.07	0.43
5:E:56:VAL:N	5:E:57:PRO:HD2	2.34	0.43
25:a:1045:C:O2	25:a:1111:A:N6	2.51	0.43
25:a:1746:A:H2'	25:a:1747:U:C6	2.53	0.43
30:f:117:LEU:HD12	30:f:176:PRO:HD2	2.01	0.43
1:A:85:U:H1'	1:A:86:G:N1	2.34	0.43
1:A:437:U:H6	1:A:437:U:C5'	2.29	0.43
1:A:1317:C:N3	19:S:37:ARG:NH1	2.54	0.43
1:A:1328:C:H2'	1:A:1329:A:O4'	2.19	0.43
24:Y:25:C:H2'	24:Y:26:G:O4'	2.19	0.43
25:a:1519:G:C6	25:a:1520:U:C4	3.07	0.43
25:a:1521:G:H2'	25:a:1522:A:C8	2.53	0.43
25:a:1545:A:H2'	25:a:1546:G:O4'	2.19	0.43
25:a:2615:U:C2	50:z:4:GLN:HA	2.54	0.43
1:A:1477:U:H2'	1:A:1478:U:C6	2.53	0.43
2:B:71:GLY:O	2:B:93:ASN:HA	2.17	0.43
11:K:97:ILE:HG22	21:U:12:PHE:HZ	1.83	0.43
27:c:165:VAL:HG21	27:c:181:MET:CE	2.49	0.43
1:A:513:C:H2'	1:A:514:C:C6	2.54	0.42
22:V:8:U:H1'	22:V:21:A:C2	2.53	0.42
38:n:4:LYS:O	38:n:8:ILE:HG12	2.18	0.42
41:q:14:VAL:HG11	41:q:20:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:A:C2	1:A:383:A:C4	3.07	0.42
1:A:1024:G:H3'	1:A:1025:U:H6	1.84	0.42
1:A:1040:U:H2'	1:A:1041:G:C8	2.54	0.42
2:B:119:THR:O	2:B:123:ASP:CB	2.58	0.42
30:f:69:LYS:HE3	30:f:69:LYS:HB3	1.86	0.42
40:p:58:ARG:HA	40:p:61:TRP:CE3	2.53	0.42
1:A:1015:G:H2'	1:A:1016:A:C8	2.53	0.42
1:A:1422:G:O2'	34:j:49:ARG:NH2	2.52	0.42
25:a:2271:G:OP1	46:v:18:ALA:HB1	2.19	0.42
25:a:2293:G:H2'	25:a:2294:G:O4'	2.18	0.42
17:Q:47:HIS:HB3	17:Q:74:THR:HG22	2.01	0.42
25:a:109:C:N3	25:a:110:G:C8	2.87	0.42
25:a:693:A:O2'	25:a:1353:A:N3	2.50	0.42
25:a:1605:C:O4'	25:a:1610:A:C6	2.73	0.42
25:a:1871:A:H2'	25:a:1872:A:C8	2.54	0.42
25:a:1932:A:H2'	25:a:1933:G:O4'	2.19	0.42
25:a:1963:U:H6	25:a:1963:U:O5'	2.02	0.42
38:n:53:THR:HB	38:n:65:THR:HB	2.01	0.42
1:A:923:A:H2'	1:A:924:C:O4'	2.20	0.42
24:Y:19:G:OP2	24:Y:20:C:N4	2.52	0.42
25:a:2233:U:H2'	25:a:2234:G:C8	2.54	0.42
33:i:4:PHE:O	40:p:64:ARG:NH1	2.50	0.42
1:A:293:G:C6	1:A:294:U:C4	3.07	0.42
1:A:1144:G:N2	1:A:1146:A:H62	2.18	0.42
16:P:46:LYS:HD2	16:P:46:LYS:HA	1.84	0.42
25:a:1519:G:C6	25:a:1520:U:N3	2.87	0.42
25:a:2458:G:O2'	25:a:2460:U:O4	2.36	0.42
1:A:622:A:C8	1:A:623:C:C6	3.07	0.42
1:A:994:A:C5	1:A:1216:A:H4'	2.54	0.42
1:A:1381:U:H2'	1:A:1382:C:O4'	2.19	0.42
2:B:66:LYS:HE3	2:B:158:PRO:HA	2.02	0.42
1:A:555:U:H2'	1:A:556:C:C6	2.55	0.42
1:A:688:G:O2'	1:A:704:A:N1	2.46	0.42
25:a:877:A:O2'	25:a:900:A:N6	2.52	0.42
1:A:5:U:H4'	1:A:6:G:O5'	2.19	0.42
1:A:1005:A:H3'	1:A:1006:G:H8	1.84	0.42
13:M:71:ARG:NH2	30:f:115:ARG:HD3	2.35	0.42
25:a:277:G:H1'	25:a:278:A:C5	2.55	0.42
25:a:696:G:O6	58:a:6213:SPM:H81	2.19	0.42
25:a:861:A:C2	25:a:917:A:C4	3.08	0.42
25:a:1536:C:H4'	25:a:1537:G:C4	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:136:ILE:HD13	30:f:136:ILE:HA	1.87	0.42
1:A:27:G:H2'	1:A:28:A:O4'	2.20	0.42
1:A:89:U:H2'	1:A:90:C:C6	2.54	0.42
1:A:664:G:H2'	1:A:666:G:OP1	2.20	0.42
1:A:1256:A:O2'	1:A:1278:G:O6	2.34	0.42
1:A:1272:G:H2'	1:A:1273:C:C6	2.54	0.42
2:B:4:VAL:HG11	2:B:9:MET:HE3	2.01	0.42
25:a:1050:A:C2	25:a:2751:G:C4	3.07	0.42
25:a:2266:A:H4'	25:a:2267:A:O5'	2.19	0.42
1:A:1127:G:H5'	1:A:1280:A:O2'	2.20	0.41
25:a:752:A:H3'	52:1:1:MET:SD	2.60	0.41
25:a:1588:G:H2'	25:a:1589:U:C6	2.54	0.41
25:a:1939:5MU:OP1	25:a:2604:PSU:O2'	2.38	0.41
25:a:2219:U:C4	25:a:2220:U:C4	3.08	0.41
30:f:95:ARG:NH2	55:4:1:MET:HE2	2.35	0.41
1:A:769:G:H4'	1:A:1513:A:H4'	2.01	0.41
2:B:157:LEU:HD13	2:B:179:LEU:HD13	2.03	0.41
5:E:85:VAL:HG23	5:E:96:MET:HE3	2.02	0.41
22:V:14:A:H3'	22:V:15:G:H8	1.84	0.41
22:Z:50:U:H2'	22:Z:51:C:O5'	2.20	0.41
25:a:12:U:O2	25:a:12:U:C2'	2.67	0.41
25:a:2636:C:H2'	25:a:2637:U:C6	2.55	0.41
25:a:2756:U:H1'	25:a:2757:A:H5''	2.02	0.41
1:A:511:C:C2	1:A:512:U:C5	3.08	0.41
10:J:32:THR:HG22	10:J:82:LYS:HG3	2.03	0.41
12:L:4:VAL:CG2	17:Q:34:TYR:HB3	2.50	0.41
15:O:88:ARG:HH12	25:a:716:A:P	2.44	0.41
1:A:83:C:O2'	1:A:86:G:N2	2.54	0.41
1:A:1144:G:H21	1:A:1146:A:H62	1.68	0.41
1:A:1316:G:N1	1:A:1319:A:OP2	2.50	0.41
44:t:54:GLN:N	44:t:55:PRO:HD2	2.35	0.41
1:A:464:U:O2'	1:A:466:A:N7	2.46	0.41
1:A:978:A:C5	1:A:1319:A:C2	3.08	0.41
24:Y:70:A:H3'	24:Y:71:C:H6	1.85	0.41
25:a:2467:C:H2'	25:a:2468:A:O4'	2.21	0.41
1:A:1085:U:H3'	1:A:1086:U:C5	2.56	0.41
24:Y:47(O):A:H2'	24:Y:47(P):U:C6	2.55	0.41
26:b:42:C:C5	30:f:66:LEU:HD22	2.55	0.41
1:A:255:G:H5'	17:Q:18:GLU:O	2.21	0.41
1:A:513:C:H2'	1:A:514:C:H6	1.85	0.41
1:A:927:G:O2'	1:A:1503:A:N7	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:40:GLU:CD	9:I:41:ARG:HH22	2.28	0.41
10:J:10:LEU:HD12	10:J:22:THR:HG23	2.02	0.41
25:a:594:U:H2'	25:a:595:C:C6	2.56	0.41
25:a:620:G:H4'	25:a:621:A:O5'	2.21	0.41
25:a:1558:C:H4'	25:a:1559:U:O5'	2.20	0.41
25:a:1824:G:O3'	27:c:247:PRO:HD3	2.20	0.41
36:l:20:LEU:HD13	45:u:81:PRO:HG2	2.01	0.41
1:A:325:A:H2'	1:A:326:G:O4'	2.21	0.41
1:A:579:A:H2'	1:A:580:C:C6	2.56	0.41
22:V:16:C:H3'	22:V:17:C:O4'	2.20	0.41
25:a:2033:A:O2'	25:a:2035:G:OP2	2.31	0.41
1:A:140:U:H2'	1:A:141:G:O4'	2.20	0.41
1:A:268:U:H2'	1:A:269:C:C6	2.56	0.41
1:A:339:C:C6	34:j:98:ARG:NH1	2.89	0.41
4:D:129:VAL:HG21	4:D:146:ARG:HH21	1.86	0.41
24:Y:47(E):C:O2'	24:Y:47(H):A:N6	2.53	0.41
25:a:285:G:C5	25:a:356:G:C6	3.09	0.41
25:a:290:U:H2'	25:a:291:G:O4'	2.20	0.41
25:a:475:C:O2	25:a:479:A:N6	2.47	0.41
25:a:1577:C:H2'	25:a:1578:U:O4'	2.21	0.41
25:a:1878:G:H2'	25:a:1879:C:O4'	2.20	0.41
1:A:405:U:O4	4:D:2:ALA:N	2.54	0.41
1:A:406:G:N7	1:A:495:A:O2'	2.40	0.41
21:U:58:LYS:O	21:U:59:LYS:C	2.63	0.41
25:a:454:A:H4'	25:a:455:C:OP2	2.21	0.41
25:a:460:A:OP1	52:l:41:ARG:NH1	2.53	0.41
25:a:2079:U:H2'	25:a:2080:A:O4'	2.21	0.41
30:f:36:LEU:HB2	30:f:89:VAL:HG22	2.03	0.41
1:A:94:G:H5''	1:A:95:C:C5	2.56	0.40
25:a:1420:A:O2'	25:a:1421:G:H5'	2.21	0.40
25:a:1425:G:H2'	25:a:1426:G:O4'	2.21	0.40
25:a:2529:G:O6	54:3:32:LYS:NZ	2.54	0.40
26:b:117:G:OP1	38:n:56:LYS:HD3	2.21	0.40
30:f:49:LEU:HD23	30:f:49:LEU:HA	1.93	0.40
1:A:299:G:H2'	1:A:300:A:C8	2.56	0.40
24:Y:14:A:H2'	24:Y:15:G:O4'	2.21	0.40
25:a:1028:A:N6	25:a:1125:G:H2'	2.36	0.40
34:j:63:VAL:HG12	34:j:107:LEU:HD11	2.03	0.40
43:s:69:ARG:NH1	43:s:74:ILE:HD13	2.35	0.40
1:A:918:A:H2'	1:A:919:A:O4'	2.20	0.40
1:A:1225:A:H2'	1:A:1226:C:C5	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:A:N6	1:A:1274:A:O2'	2.53	0.40
24:Y:28:U:H2'	24:Y:29:C:C6	2.57	0.40
22:Z:71:C:H2'	22:Z:72:A:C8	2.56	0.40
25:a:546:U:O2	25:a:546:U:O4'	2.40	0.40
25:a:875:G:C6	25:a:876:C:N3	2.90	0.40
25:a:1370:C:H2'	25:a:1371:G:O4'	2.21	0.40
25:a:2082:A:H2'	25:a:2083:G:O4'	2.22	0.40
38:n:94:ARG:HD2	38:n:97:PHE:O	2.21	0.40
1:A:1:A:H62	1:A:2:A:N6	2.20	0.40
1:A:868:C:H2'	1:A:869:G:O4'	2.21	0.40
2:B:79:ALA:HB2	2:B:207:ILE:HD11	2.04	0.40
13:M:83:LEU:HD21	19:S:65:GLU:CB	2.51	0.40
22:Z:67:C:O2'	22:Z:68:C:H5'	2.22	0.40
25:a:247:G:H4'	25:a:386:G:C5	2.57	0.40
25:a:861:A:H2'	25:a:862:G:O4'	2.22	0.40
25:a:1856:U:H2'	25:a:1857:G:O4'	2.22	0.40
1:A:392:C:OP1	16:P:8:ARG:NH2	2.55	0.40
1:A:1202:U:H2'	1:A:1203:C:O4'	2.22	0.40
4:D:99:ASP:OD2	4:D:115:ARG:HA	2.21	0.40
25:a:638:G:H2'	25:a:639:U:C6	2.56	0.40
26:b:14:U:OP2	26:b:70:C:O2'	2.39	0.40
26:b:90:C:H5''	36:l:18:ARG:HG2	2.03	0.40
41:q:6:GLN:HG3	41:q:39:LEU:HD11	2.03	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	
2	B	222/241 (92%)	203 (91%)	19 (9%)	0	100	100
3	C	204/233 (88%)	199 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	203/206 (98%)	192 (95%)	10 (5%)	1 (0%)	25	44
5	E	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
6	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
7	G	151/179 (84%)	145 (96%)	6 (4%)	0	100	100
8	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	I	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	J	96/103 (93%)	94 (98%)	1 (1%)	1 (1%)	13	25
11	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
12	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
13	M	113/118 (96%)	112 (99%)	1 (1%)	0	100	100
14	N	98/101 (97%)	98 (100%)	0	0	100	100
15	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	P	79/82 (96%)	78 (99%)	1 (1%)	0	100	100
17	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
18	R	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
19	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
20	T	84/87 (97%)	84 (100%)	0	0	100	100
21	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
27	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
28	d	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
29	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
30	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
31	g	171/177 (97%)	164 (96%)	7 (4%)	0	100	100
32	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
33	i	140/142 (99%)	140 (100%)	0	0	100	100
34	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
35	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
36	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
37	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
38	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
39	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
41	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
42	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
43	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
44	t	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
45	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
46	v	82/85 (96%)	78 (95%)	4 (5%)	0	100	100
47	w	75/78 (96%)	75 (100%)	0	0	100	100
48	x	59/63 (94%)	59 (100%)	0	0	100	100
49	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
51	0	49/55 (89%)	49 (100%)	0	0	100	100
52	1	44/46 (96%)	44 (100%)	0	0	100	100
53	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	3	36/38 (95%)	36 (100%)	0	0	100	100
55	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
All	All	5483/5913 (93%)	5321 (97%)	160 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL
4	D	25	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	182 (98%)	4 (2%)	47	73
3	C	170/190 (90%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	172/173 (99%)	169 (98%)	3 (2%)	56	79
5	E	119/126 (94%)	118 (99%)	1 (1%)	79	91
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	125 (99%)	1 (1%)	79	91
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	104 (99%)	1 (1%)	73	88
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	89/98 (91%)	88 (99%)	1 (1%)	70	87
12	L	102/103 (99%)	101 (99%)	1 (1%)	73	88
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	56 (98%)	1 (2%)	54	78
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	64 (98%)	1 (2%)	60	82
21	U	60/61 (98%)	58 (97%)	2 (3%)	33	59
27	c	216/218 (99%)	215 (100%)	1 (0%)	86	95
28	d	163/163 (100%)	161 (99%)	2 (1%)	67	86
29	e	165/165 (100%)	165 (100%)	0	100	100
30	f	148/150 (99%)	142 (96%)	6 (4%)	26	50
31	g	134/138 (97%)	132 (98%)	2 (2%)	60	82
32	h	32/114 (28%)	32 (100%)	0	100	100
33	i	116/116 (100%)	115 (99%)	1 (1%)	75	90
34	j	104/104 (100%)	104 (100%)	0	100	100
35	k	103/103 (100%)	103 (100%)	0	100	100
36	l	107/107 (100%)	107 (100%)	0	100	100
37	m	98/103 (95%)	98 (100%)	0	100	100
38	n	86/87 (99%)	80 (93%)	6 (7%)	12	26
39	o	99/100 (99%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	p	89/90 (99%)	89 (100%)	0	100	100
41	q	84/84 (100%)	84 (100%)	0	100	100
42	r	93/93 (100%)	92 (99%)	1 (1%)	70	87
43	s	80/84 (95%)	80 (100%)	0	100	100
44	t	83/85 (98%)	83 (100%)	0	100	100
45	u	78/78 (100%)	78 (100%)	0	100	100
46	v	61/63 (97%)	60 (98%)	1 (2%)	58	80
47	w	67/68 (98%)	67 (100%)	0	100	100
48	x	54/55 (98%)	53 (98%)	1 (2%)	52	77
49	y	48/49 (98%)	48 (100%)	0	100	100
50	z	47/48 (98%)	47 (100%)	0	100	100
51	0	46/49 (94%)	46 (100%)	0	100	100
52	1	38/38 (100%)	38 (100%)	0	100	100
53	2	51/52 (98%)	51 (100%)	0	100	100
54	3	34/34 (100%)	34 (100%)	0	100	100
55	4	55/62 (89%)	52 (94%)	3 (6%)	18	37
All	All	4572/4825 (95%)	4532 (99%)	40 (1%)	74	90

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	36	ASN
2	B	118	GLU
2	B	133	GLU
2	B	161	LEU
4	D	25	VAL
4	D	44	ARG
4	D	99	ASP
5	E	26	LYS
7	G	2	PRO
9	I	59	GLU
11	K	129	VAL
12	L	88	LYS
18	R	74	HIS
20	T	43	ASP
21	U	60	LEU

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Mol	Chain	Res	Type
21	U	63	GLU
27	c	37	ASN
28	d	2	ILE
28	d	32	ASN
30	f	32	GLU
30	f	50	LEU
30	f	85	ILE
30	f	120	LYS
30	f	136	ILE
30	f	150	ARG
31	g	43	VAL
31	g	48	ASN
33	i	9	GLU
38	n	13	ARG
38	n	16	ARG
38	n	45	SER
38	n	56	LYS
38	n	84	GLU
38	n	116	GLN
42	r	109	ASP
46	v	10	THR
48	x	6	LEU
55	4	13	THR
55	4	17	SER
55	4	24	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	ASN
2	B	103	ASN
2	B	170	HIS
2	B	177	ASN
2	B	178	ASN
3	C	102	ASN
3	C	139	GLN
3	C	140	ASN
4	D	40	GLN
4	D	41	HIS
4	D	54	GLN
4	D	136	GLN
5	E	82	GLN

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Mol	Chain	Res	Type
5	E	132	ASN
6	F	46	GLN
7	G	9	GLN
7	G	68	ASN
7	G	86	GLN
8	H	21	ASN
9	I	4	ASN
9	I	25	ASN
9	I	31	ASN
9	I	32	GLN
10	J	58	ASN
12	L	112	GLN
13	M	8	ASN
14	N	4	GLN
15	O	35	GLN
15	O	40	GLN
18	R	52	GLN
19	S	14	HIS
19	S	52	HIS
19	S	83	HIS
20	T	3	ASN
20	T	13	GLN
27	c	25	HIS
27	c	90	ASN
29	e	92	HIS
31	g	30	ASN
31	g	73	ASN
32	h	20	ASN
33	i	80	HIS
33	i	86	GLN
34	j	5	GLN
35	k	104	GLN
36	l	13	HIS
36	l	97	GLN
37	m	9	GLN
37	m	18	GLN
37	m	107	ASN
38	n	100	HIS
39	o	66	ASN
40	p	52	GLN
40	p	81	ASN
41	q	6	GLN

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Mol	Chain	Res	Type
41	q	12	HIS
42	r	9	HIS
43	s	28	ASN
43	s	70	HIS
44	t	53	ASN
48	x	15	ASN
48	x	27	ASN
48	x	39	GLN
48	x	45	GLN
55	4	20	ASN
55	4	30	HIS
55	4	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1527/1542 (99%)	227 (14%)	16 (1%)
22	V	75/76 (98%)	31 (41%)	2 (2%)
22	Z	75/76 (98%)	29 (38%)	4 (5%)
23	X	10/24 (41%)	0	0
24	Y	92/93 (98%)	19 (20%)	1 (1%)
25	a	2749/2904 (94%)	328 (11%)	0
26	b	118/120 (98%)	11 (9%)	0
All	All	4646/4835 (96%)	645 (13%)	23 (0%)

All (645) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	4	U
1	A	5	U
1	A	6	G
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	71	A
1	A	74	A

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Mol	Chain	Res	Type
1	A	75	G
1	A	76	G
1	A	79	G
1	A	80	A
1	A	81	A
1	A	82	G
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	87	C
1	A	88	U
1	A	91	U
1	A	94	G
1	A	95	C
1	A	97	G
1	A	122	G
1	A	130	A
1	A	131	A
1	A	141	G
1	A	143	A
1	A	144	G
1	A	163	C
1	A	164	G
1	A	177	G
1	A	182	A
1	A	183	C
1	A	197	A
1	A	200	G
1	A	202	G
1	A	204	G
1	A	205	A
1	A	210	C
1	A	211	G
1	A	212	G
1	A	213	G
1	A	214	C
1	A	215	C
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G

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Mol	Chain	Res	Type
1	A	251	G
1	A	258	G
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	339	C
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	376	G
1	A	384	G
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	416	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	436	C
1	A	437	U
1	A	438	U
1	A	453	G
1	A	457	G
1	A	458	U
1	A	459	A
1	A	463	U
1	A	467	U
1	A	468	A
1	A	469	C
1	A	475	C
1	A	477	C
1	A	478	A

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Mol	Chain	Res	Type
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	495	A
1	A	497	G
1	A	500	G
1	A	511	C
1	A	518	C
1	A	531	U
1	A	547	A
1	A	559	A
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	596	A
1	A	633	G
1	A	650	G
1	A	653	U
1	A	665	A
1	A	671	G
1	A	718	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	734	G
1	A	742	G
1	A	746	A
1	A	747	A
1	A	748	G
1	A	755	G
1	A	758	C
1	A	774	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	887	G
1	A	890	G

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Mol	Chain	Res	Type
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	965	U
1	A	966	2MG
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	981	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1009	U
1	A	1027	C
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1034	G
1	A	1035	A
1	A	1036	A
1	A	1042	A
1	A	1043	G
1	A	1044	A
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1159	U
1	A	1171	A
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C

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Mol	Chain	Res	Type
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1256	A
1	A	1260	G
1	A	1275	A
1	A	1280	A
1	A	1285	A
1	A	1286	U
1	A	1287	A
1	A	1290	G
1	A	1300	G
1	A	1302	C
1	A	1317	C
1	A	1320	C
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1368	A
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1406	U
1	A	1419	G
1	A	1432	G
1	A	1441	A
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1458	G
1	A	1487	G
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1503	A
1	A	1506	U

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Mol	Chain	Res	Type
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
22	V	5	G
22	V	7	G
22	V	8	U
22	V	9	G
22	V	10	G
22	V	11	A
22	V	13	C
22	V	17(A)	U
22	V	18	G
22	V	19	G
22	V	20	U
22	V	21	A
22	V	26	G
22	V	32	C
22	V	33	U
22	V	34	C
22	V	35	A
22	V	36	U
22	V	37	A
22	V	38	A
22	V	43	A
22	V	44	A
22	V	46	G
22	V	48	C
22	V	49	G
22	V	56	C
22	V	58	A
22	V	65	C
22	V	68	C
22	V	72	A
22	V	76	A
24	Y	3	U
24	Y	6	G
24	Y	7	G
24	Y	13	G
24	Y	14	A
24	Y	16	A
24	Y	18	G

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Mol	Chain	Res	Type
24	Y	20(B)	G
24	Y	25	C
24	Y	32	RSP
24	Y	40	G
24	Y	45	A
24	Y	47(C)	G
24	Y	47(J)	G
24	Y	47(K)	C
24	Y	48	C
24	Y	70	A
24	Y	71	C
24	Y	74	C
22	Z	6	G
22	Z	7	G
22	Z	8	U
22	Z	9	G
22	Z	14	A
22	Z	16	C
22	Z	17	C
22	Z	17(A)	U
22	Z	18	G
22	Z	19	G
22	Z	21	A
22	Z	22	G
22	Z	31	G
22	Z	47	U
22	Z	48	C
22	Z	49	G
22	Z	50	U
22	Z	51	C
22	Z	52	G
22	Z	53	G
22	Z	54	U
22	Z	55	U
22	Z	58	A
22	Z	65	C
22	Z	66	C
22	Z	68	C
22	Z	69	C
22	Z	71	C
22	Z	76	A
25	a	10	A

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Mol	Chain	Res	Type
25	a	34	U
25	a	42	A
25	a	45	G
25	a	58	G
25	a	61	C
25	a	71	A
25	a	74	A
25	a	75	G
25	a	84	A
25	a	101	A
25	a	102	U
25	a	103	A
25	a	118	A
25	a	119	A
25	a	120	U
25	a	139	U
25	a	142	A
25	a	163	C
25	a	181	A
25	a	196	A
25	a	199	A
25	a	215	G
25	a	216	A
25	a	222	A
25	a	248	G
25	a	264	C
25	a	265	A
25	a	272	A
25	a	277	G
25	a	278	A
25	a	282	A
25	a	285	G
25	a	289	G
25	a	294	A
25	a	311	A
25	a	329	G
25	a	330	A
25	a	345	A
25	a	357	C
25	a	361	G
25	a	362	A
25	a	386	G

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Mol	Chain	Res	Type
25	a	396	G
25	a	405	U
25	a	411	G
25	a	412	A
25	a	455	C
25	a	481	G
25	a	491	G
25	a	504	A
25	a	505	A
25	a	509	C
25	a	530	G
25	a	532	A
25	a	544	C
25	a	545	U
25	a	547	A
25	a	548	G
25	a	549	G
25	a	563	A
25	a	564	C
25	a	573	U
25	a	575	A
25	a	586	A
25	a	603	A
25	a	614	A
25	a	615	U
25	a	627	A
25	a	637	A
25	a	645	C
25	a	647	G
25	a	654	A
25	a	655	A
25	a	664	G
25	a	686	U
25	a	717	C
25	a	721	A
25	a	730	A
25	a	732	C
25	a	738	G
25	a	747	5MU
25	a	761	A
25	a	764	A
25	a	765	C

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Mol	Chain	Res	Type
25	a	775	G
25	a	776	G
25	a	782	A
25	a	784	G
25	a	785	G
25	a	805	G
25	a	806	C
25	a	812	C
25	a	827	U
25	a	828	U
25	a	845	A
25	a	846	U
25	a	847	U
25	a	859	G
25	a	879	G
25	a	881	G
25	a	883	G
25	a	884	U
25	a	888	C
25	a	890	C
25	a	891	G
25	a	895	U
25	a	896	A
25	a	897	C
25	a	898	C
25	a	899	A
25	a	910	A
25	a	914	G
25	a	915	C
25	a	931	U
25	a	934	U
25	a	946	C
25	a	958	U
25	a	961	C
25	a	974	G
25	a	983	A
25	a	996	A
25	a	1005	C
25	a	1012	U
25	a	1013	C
25	a	1022	G
25	a	1033	U

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Mol	Chain	Res	Type
25	a	1040	A
25	a	1041	G
25	a	1046	A
25	a	1047	G
25	a	1048	A
25	a	1051	G
25	a	1108	U
25	a	1111	A
25	a	1112	G
25	a	1115	G
25	a	1116	G
25	a	1122	G
25	a	1128	G
25	a	1129	A
25	a	1130	U
25	a	1132	U
25	a	1133	A
25	a	1135	C
25	a	1142	A
25	a	1169	A
25	a	1171	G
25	a	1187	G
25	a	1250	G
25	a	1253	A
25	a	1256	G
25	a	1271	G
25	a	1272	A
25	a	1289	C
25	a	1301	A
25	a	1303	G
25	a	1321	A
25	a	1344	U
25	a	1345	C
25	a	1352	U
25	a	1365	A
25	a	1379	U
25	a	1383	A
25	a	1411	U
25	a	1416	G
25	a	1417	C
25	a	1419	A
25	a	1421	G

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Mol	Chain	Res	Type
25	a	1428	C
25	a	1452	G
25	a	1453	A
25	a	1482	G
25	a	1493	C
25	a	1494	A
25	a	1509	A
25	a	1510	G
25	a	1515	A
25	a	1524	G
25	a	1529	G
25	a	1534	U
25	a	1535	A
25	a	1536	C
25	a	1537	G
25	a	1559	U
25	a	1566	A
25	a	1569	A
25	a	1578	U
25	a	1583	A
25	a	1584	U
25	a	1585	C
25	a	1586	A
25	a	1608	A
25	a	1609	A
25	a	1634	A
25	a	1647	U
25	a	1648	U
25	a	1674	G
25	a	1715	G
25	a	1729	U
25	a	1730	C
25	a	1731	G
25	a	1732	C
25	a	1738	G
25	a	1739	A
25	a	1750	G
25	a	1758	U
25	a	1764	C
25	a	1773	A
25	a	1782	U
25	a	1791	A

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Mol	Chain	Res	Type
25	a	1800	C
25	a	1808	A
25	a	1816	C
25	a	1829	A
25	a	1842	G
25	a	1847	A
25	a	1848	A
25	a	1858	A
25	a	1870	C
25	a	1871	A
25	a	1872	A
25	a	1873	G
25	a	1906	G
25	a	1929	G
25	a	1930	G
25	a	1937	A
25	a	1938	A
25	a	1955	U
25	a	1965	C
25	a	1966	A
25	a	1967	C
25	a	1970	A
25	a	1971	U
25	a	1972	G
25	a	1991	U
25	a	1993	U
25	a	2023	C
25	a	2030	6MZ
25	a	2031	A
25	a	2033	A
25	a	2043	C
25	a	2055	C
25	a	2056	G
25	a	2060	A
25	a	2061	G
25	a	2062	A
25	a	2069	G7M
25	a	2198	A
25	a	2204	G
25	a	2211	A
25	a	2225	A
25	a	2238	G

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Mol	Chain	Res	Type
25	a	2239	G
25	a	2268	A
25	a	2273	A
25	a	2283	C
25	a	2287	A
25	a	2288	A
25	a	2305	U
25	a	2308	G
25	a	2312	U
25	a	2322	A
25	a	2325	G
25	a	2335	A
25	a	2336	A
25	a	2347	C
25	a	2361	G
25	a	2371	G
25	a	2377	A
25	a	2383	G
25	a	2385	C
25	a	2396	G
25	a	2402	U
25	a	2403	C
25	a	2406	A
25	a	2425	A
25	a	2429	G
25	a	2430	A
25	a	2431	U
25	a	2435	A
25	a	2440	C
25	a	2441	U
25	a	2448	A
25	a	2470	G
25	a	2476	A
25	a	2478	A
25	a	2491	U
25	a	2502	G
25	a	2505	G
25	a	2518	A
25	a	2520	C
25	a	2529	G
25	a	2535	G
25	a	2547	A

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Mol	Chain	Res	Type
25	a	2556	C
25	a	2566	A
25	a	2567	G
25	a	2573	C
25	a	2585	U
25	a	2602	A
25	a	2609	U
25	a	2613	U
25	a	2629	U
25	a	2663	G
25	a	2688	G
25	a	2689	U
25	a	2690	U
25	a	2713	U
25	a	2714	G
25	a	2716	C
25	a	2726	A
25	a	2733	A
25	a	2744	G
25	a	2748	A
25	a	2765	A
25	a	2778	A
25	a	2795	C
25	a	2798	U
25	a	2799	A
25	a	2818	U
25	a	2820	A
25	a	2821	A
25	a	2835	A
25	a	2861	U
25	a	2884	U
25	a	2899	A
25	a	2901	C
26	b	13	G
26	b	24	G
26	b	33	G
26	b	35	C
26	b	56	G
26	b	67	G
26	b	89	U
26	b	90	C
26	b	99	A

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Mol	Chain	Res	Type
26	b	105	G
26	b	109	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	83	C
1	A	199	A
1	A	328	C
1	A	410	G
1	A	429	U
1	A	437	U
1	A	438	U
1	A	884	U
1	A	1026	G
1	A	1034	G
1	A	1035	A
1	A	1094	G
1	A	1124	G
1	A	1319	A
1	A	1397	C
22	V	7	G
22	V	36	U
24	Y	13	G
22	Z	7	G
22	Z	17(A)	U
22	Z	18	G
22	Z	48	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

45 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
25	2MG	a	1835	25	18,26,27	1.03	2 (11%)	16,38,41	0.72	0
1	PSU	A	516	56,1	18,21,22	0.91	1 (5%)	22,30,33	0.75	0
24	4SU	Y	8	24	18,21,22	0.20	0	26,30,33	0.36	0
24	PSU	Y	55	24	18,21,22	0.83	1 (5%)	22,30,33	0.61	0
28	MEQ	d	150	28	8,9,10	0.60	0	5,10,12	1.02	0
25	PSU	a	2457	25	18,21,22	0.99	1 (5%)	22,30,33	0.87	0
25	OMU	a	2552	25	19,22,23	0.53	0	26,31,34	0.85	1 (3%)
24	RSP	Y	32	24	17,21,22	0.22	0	22,30,33	0.29	0
11	IAS	K	119	11	6,7,8	0.92	0	6,8,10	1.01	0
25	PSU	a	2504	25	18,21,22	0.86	1 (5%)	22,30,33	0.90	1 (4%)
1	2MG	A	966	1	18,26,27	1.12	2 (11%)	16,38,41	0.71	0
1	MA6	A	1518	1	18,26,27	0.85	0	19,38,41	0.50	0
24	H2U	Y	20(A)	24	18,21,22	0.57	0	21,30,33	0.77	1 (4%)
25	PSU	a	955	25	18,21,22	0.90	1 (5%)	22,30,33	0.88	1 (4%)
25	6MZ	a	1618	25	18,25,26	0.69	0	16,36,39	0.91	1 (6%)
25	5MC	a	1962	25	18,22,23	0.51	0	26,32,35	0.71	1 (3%)
25	PSU	a	2580	25	18,21,22	1.01	1 (5%)	22,30,33	0.90	1 (4%)
25	PSU	a	746	56,25	18,21,22	1.06	2 (11%)	22,30,33	0.72	0
25	2MA	a	2503	56,25	19,25,26	0.95	0	21,37,40	1.60	4 (19%)
1	5MC	A	967	1	18,22,23	0.36	0	26,32,35	0.63	0
1	2MG	A	1516	1	18,26,27	1.04	3 (16%)	16,38,41	0.85	0
25	3TD	a	1915	25	18,22,23	0.93	1 (5%)	22,32,35	0.77	1 (4%)
1	MA6	A	1519	1	18,26,27	0.84	1 (5%)	19,38,41	0.66	0
25	1MG	a	745	25	18,26,27	1.09	2 (11%)	19,39,42	0.91	0
25	2MG	a	2445	25	18,26,27	1.25	3 (16%)	16,38,41	0.75	0
24	T6A	Y	37	24	27,34,35	0.87	2 (7%)	29,49,52	0.91	0
25	5MU	a	1939	25	19,22,23	0.52	0	28,32,35	0.60	0
25	G7M	a	2069	25	20,26,27	1.35	3 (15%)	17,39,42	0.77	0
25	PSU	a	1917	25	18,21,22	0.82	1 (5%)	22,30,33	1.11	2 (9%)
25	OMG	a	2251	22,25	18,26,27	0.95	2 (11%)	19,38,41	0.74	1 (5%)
25	PSU	a	2604	25	18,21,22	0.77	1 (5%)	22,30,33	1.07	2 (9%)
25	PSU	a	1911	25	18,21,22	0.86	1 (5%)	22,30,33	0.78	0
1	5MC	A	1407	1	18,22,23	0.46	0	26,32,35	0.75	1 (3%)
25	H2U	a	2449	25	18,21,22	0.89	2 (11%)	21,30,33	1.18	3 (14%)
25	OMC	a	2498	56,25	19,22,23	0.37	0	26,31,34	0.47	0
1	UR3	A	1498	1	19,22,23	0.46	0	26,32,35	0.76	0
25	5MU	a	747	25	19,22,23	0.41	0	28,32,35	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	6MZ	a	2030	25	18,25,26	0.82	0	16,36,39	0.70	0
12	D2T	L	89	12	7,9,10	1.06	0	6,11,13	1.89	4 (66%)
25	PSU	a	2605	25	18,21,22	1.02	2 (11%)	22,30,33	1.21	2 (9%)
1	2MG	A	1207	1	18,26,27	1.07	2 (11%)	16,38,41	0.85	0
36	4D4	l	81	36	9,11,12	0.45	0	8,13,15	0.93	1 (12%)
1	G7M	A	527	1	20,26,27	1.23	3 (15%)	17,39,42	0.71	0
1	4OC	A	1402	56,1	20,23,24	0.46	0	26,32,35	0.53	0
24	5MU	Y	54	24	19,22,23	0.29	0	28,32,35	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	2MG	a	1835	25	-	0/5/27/28	0/3/3/3
1	PSU	A	516	56,1	-	0/7/25/26	0/2/2/2
24	4SU	Y	8	24	-	0/7/25/26	0/2/2/2
24	PSU	Y	55	24	-	1/7/25/26	0/2/2/2
28	MEQ	d	150	28	-	2/8/9/11	-
25	PSU	a	2457	25	-	0/7/25/26	0/2/2/2
25	OMU	a	2552	25	-	0/9/27/28	0/2/2/2
24	RSP	Y	32	24	-	2/7/25/26	0/2/2/2
11	IAS	K	119	11	-	1/7/7/8	-
25	PSU	a	2504	25	-	2/7/25/26	0/2/2/2
1	2MG	A	966	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
24	H2U	Y	20(A)	24	-	3/7/38/39	0/2/2/2
25	PSU	a	955	25	-	0/7/25/26	0/2/2/2
25	6MZ	a	1618	25	-	0/5/27/28	0/3/3/3
25	5MC	a	1962	25	-	1/7/25/26	0/2/2/2
25	PSU	a	2580	25	-	0/7/25/26	0/2/2/2
25	PSU	a	746	56,25	-	1/7/25/26	0/2/2/2
25	2MA	a	2503	56,25	-	2/3/25/26	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
25	3TD	a	1915	25	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3
25	1MG	a	745	25	-	0/3/25/26	0/3/3/3
25	2MG	a	2445	25	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	T6A	Y	37	24	-	6/19/41/42	0/3/3/3
25	5MU	a	1939	25	-	0/7/25/26	0/2/2/2
25	G7M	a	2069	25	-	2/3/25/26	0/3/3/3
25	PSU	a	1917	25	-	0/7/25/26	0/2/2/2
25	OMG	a	2251	22,25	-	1/5/27/28	0/3/3/3
25	PSU	a	2604	25	-	0/7/25/26	0/2/2/2
25	PSU	a	1911	25	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
25	H2U	a	2449	25	-	0/7/38/39	0/2/2/2
25	OMC	a	2498	56,25	-	0/9/27/28	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
25	5MU	a	747	25	-	0/7/25/26	0/2/2/2
25	6MZ	a	2030	25	-	2/5/27/28	0/3/3/3
12	D2T	L	89	12	-	4/7/12/14	-
25	PSU	a	2605	25	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
36	4D4	l	81	36	-	1/11/12/14	-
1	G7M	A	527	1	-	1/3/25/26	0/3/3/3
1	4OC	A	1402	56,1	-	0/9/29/30	0/2/2/2
24	5MU	Y	54	24	-	0/7/25/26	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	2069	G7M	C5-C6	-3.62	1.36	1.45
25	a	2445	2MG	C5-C6	-3.60	1.40	1.47
25	a	1915	3TD	C6-C5	3.50	1.39	1.35
25	a	2069	G7M	C8-N9	3.29	1.39	1.33
25	a	2457	PSU	C6-C5	3.19	1.39	1.35
1	A	527	G7M	C8-N9	3.13	1.38	1.33
24	Y	55	PSU	C6-C5	3.11	1.38	1.35
1	A	527	G7M	C8-N7	2.98	1.38	1.33
25	a	2504	PSU	C6-C5	2.98	1.38	1.35
25	a	2580	PSU	C6-C5	2.96	1.38	1.35
1	A	516	PSU	C6-C5	2.91	1.38	1.35
1	A	966	2MG	C5-C6	-2.89	1.41	1.47
25	a	746	PSU	C4-C5	-2.84	1.36	1.44
25	a	1911	PSU	C6-C5	2.81	1.38	1.35
1	A	1516	2MG	C5-C6	-2.78	1.41	1.47
1	A	1207	2MG	C5-C6	-2.76	1.41	1.47
25	a	2069	G7M	C8-N7	2.68	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	G7M	C5-C6	-2.68	1.38	1.45
25	a	1835	2MG	C5-C6	-2.66	1.42	1.47
25	a	1917	PSU	C6-C5	2.58	1.38	1.35
25	a	2605	PSU	C6-C5	2.56	1.38	1.35
25	a	2604	PSU	C6-C5	2.54	1.38	1.35
25	a	2449	H2U	C2-N3	-2.54	1.33	1.38
25	a	745	1MG	C5-C4	-2.45	1.36	1.43
25	a	955	PSU	C6-C5	2.37	1.38	1.35
25	a	2445	2MG	C8-N7	-2.30	1.31	1.35
25	a	745	1MG	C5-C6	-2.28	1.40	1.47
25	a	1835	2MG	C5-C4	-2.28	1.37	1.43
25	a	2251	OMG	C5-C4	-2.26	1.37	1.43
25	a	2445	2MG	C5-C4	-2.22	1.37	1.43
25	a	2605	PSU	C4-C5	-2.21	1.37	1.44
1	A	1519	MA6	C8-N7	-2.21	1.30	1.34
25	a	2251	OMG	C5-C6	-2.21	1.42	1.47
1	A	1516	2MG	C5-C4	-2.19	1.37	1.43
24	Y	37	T6A	C8-N7	-2.16	1.30	1.34
1	A	966	2MG	C8-N7	-2.15	1.31	1.35
24	Y	37	T6A	C2'-C1'	-2.11	1.50	1.53
1	A	1207	2MG	C5-C4	-2.08	1.37	1.43
25	a	746	PSU	C6-C5	2.05	1.37	1.35
1	A	1516	2MG	C8-N7	-2.04	1.31	1.35
25	a	2449	H2U	C2-N1	-2.02	1.32	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	2503	2MA	C5-C6-N1	-4.16	118.28	121.01
25	a	2503	2MA	C5-C6-N6	4.05	126.51	120.35
25	a	1917	PSU	C5-C6-N1	-2.69	118.08	122.11
25	a	2605	PSU	C5-C6-N1	-2.68	118.10	122.11
25	a	2449	H2U	N3-C2-N1	2.67	119.48	116.65
25	a	2604	PSU	C5-C6-N1	-2.46	118.42	122.11
25	a	2552	OMU	C2'-C1'-N1	-2.43	109.52	114.22
25	a	2449	H2U	O2-C2-N1	-2.38	120.12	123.11
12	L	89	D2T	O-C-CA	-2.37	118.56	124.78
12	L	89	D2T	OD2-CG-CB	2.37	118.27	113.15
25	a	2503	2MA	C2-N1-C6	2.33	121.72	118.08
25	a	2503	2MA	N3-C2-N1	-2.31	121.51	125.73
25	a	2580	PSU	C3'-C2'-C1'	2.29	104.31	101.64
1	A	1407	5MC	C5-C6-N1	-2.27	121.00	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	20(A)	H2U	C4-N3-C2	-2.24	123.93	125.79
12	L	89	D2T	OD1-CG-CB	-2.24	117.75	122.44
25	a	955	PSU	C5-C6-N1	-2.20	118.80	122.11
25	a	2449	H2U	C4-N3-C2	-2.16	124.00	125.79
12	L	89	D2T	CB-CA-N	2.16	113.71	109.10
25	a	2251	OMG	O6-C6-C5	2.16	128.59	124.37
25	a	2604	PSU	C2'-C3'-C4'	-2.14	98.48	102.64
25	a	1917	PSU	C6-C5-C4	2.14	119.69	118.20
36	l	81	4D4	O-C-CA	-2.14	119.18	124.78
25	a	2504	PSU	C2'-C3'-C4'	-2.12	98.53	102.64
25	a	1915	3TD	O4-C4-N3	-2.11	116.43	120.30
25	a	1618	6MZ	C2-N1-C6	2.10	118.39	116.59
25	a	2605	PSU	C4-N3-C2	-2.10	123.31	126.34
25	a	1962	5MC	C5-C6-N1	-2.04	121.24	123.34

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	CA-CB-CG-OD1
24	Y	32	RSP	C3'-C4'-C5'-O5'
24	Y	32	RSP	O4'-C4'-C5'-O5'
24	Y	37	T6A	N11-C12-C14-O14
24	Y	37	T6A	C13-C12-C14-O14
24	Y	37	T6A	C13-C12-C14-C15
25	a	2251	OMG	C1'-C2'-O2'-CM2
25	a	2030	6MZ	O4'-C4'-C5'-O5'
25	a	2030	6MZ	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
28	d	150	MEQ	NE2-CD-CG-CB
28	d	150	MEQ	OE1-CD-CG-CB
24	Y	37	T6A	N11-C12-C13-ODB
24	Y	37	T6A	N11-C12-C13-ODA
25	a	2504	PSU	O4'-C4'-C5'-O5'
24	Y	20(A)	H2U	C2'-C1'-N1-C6
24	Y	37	T6A	N11-C12-C14-C15
1	A	1519	MA6	C3'-C4'-C5'-O5'
12	L	89	D2T	CA-CB-CG-OD2
25	a	2503	2MA	O4'-C4'-C5'-O5'
11	K	119	IAS	O-C-CA-N
12	L	89	D2T	SB-CB-CG-OD2
24	Y	20(A)	H2U	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
24	Y	20(A)	H2U	C2'-C1'-N1-C2
25	a	2503	2MA	C4'-C5'-O5'-P
12	L	89	D2T	CG-CB-SB-CB1
24	Y	55	PSU	O4'-C1'-C5-C6
25	a	746	PSU	O4'-C1'-C5-C6
25	a	2069	G7M	O4'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
25	a	2504	PSU	C3'-C4'-C5'-O5'
36	l	81	4D4	O-C-CA-CB
25	a	2069	G7M	C4'-C5'-O5'-P
25	a	1962	5MC	O4'-C1'-N1-C6
25	a	2445	2MG	C3'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Y	8	4SU	1	0
24	Y	37	T6A	1	0
25	a	1939	5MU	2	0
25	a	2251	OMG	1	0
25	a	2604	PSU	1	0
25	a	2030	6MZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 329 ligands modelled in this entry, 316 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	PUT	a	6215	-	5,5,5	0.15	0	4,4,4	0.20	0
59	PUT	a	6217	-	5,5,5	0.13	0	4,4,4	0.16	0
57	SPD	a	6207	-	9,9,9	0.27	0	8,8,8	0.30	0
57	SPD	a	6210	-	9,9,9	0.22	0	8,8,8	0.21	0
58	SPM	a	6213	-	13,13,13	0.26	0	12,12,12	0.22	0
57	SPD	a	6208	-	9,9,9	0.18	0	8,8,8	0.16	0
57	SPD	a	6211	-	9,9,9	0.21	0	8,8,8	0.27	0
59	PUT	a	6218	-	5,5,5	0.24	0	4,4,4	0.20	0
59	PUT	a	6216	-	5,5,5	0.16	0	4,4,4	0.25	0
57	SPD	a	6209	-	9,9,9	0.26	0	8,8,8	0.41	0
57	SPD	a	6212	-	9,9,9	0.19	0	8,8,8	0.29	0
59	PUT	a	6219	-	5,5,5	0.20	0	4,4,4	0.24	0
59	PUT	a	6214	-	5,5,5	0.19	0	4,4,4	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	a	6215	-	-	0/3/3/3	-
59	PUT	a	6217	-	-	1/3/3/3	-
57	SPD	a	6207	-	-	2/7/7/7	-
57	SPD	a	6210	-	-	2/7/7/7	-
58	SPM	a	6213	-	-	2/11/11/11	-
57	SPD	a	6208	-	-	0/7/7/7	-
57	SPD	a	6211	-	-	0/7/7/7	-
59	PUT	a	6218	-	-	0/3/3/3	-
59	PUT	a	6216	-	-	0/3/3/3	-
57	SPD	a	6209	-	-	0/7/7/7	-
57	SPD	a	6212	-	-	0/7/7/7	-
59	PUT	a	6219	-	-	0/3/3/3	-
59	PUT	a	6214	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	a	6207	SPD	C3-C4-C5-N6
58	a	6213	SPM	N10-C11-C12-C13
59	a	6217	PUT	C1-C2-C3-C4
58	a	6213	SPM	N5-C6-C7-C8
57	a	6210	SPD	C2-C3-C4-C5
57	a	6210	SPD	N6-C7-C8-C9
57	a	6207	SPD	C4-C5-N6-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	a	6207	SPD	1	0
58	a	6213	SPM	1	0
57	a	6211	SPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

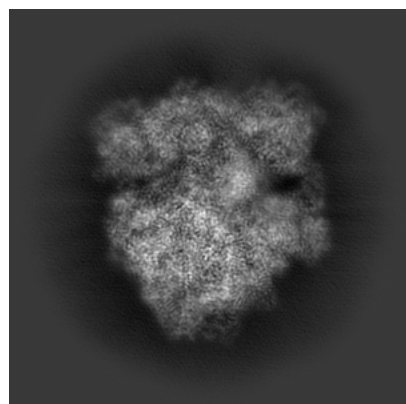
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51758. These allow visual inspection of the internal detail of the map and identification of artifacts.

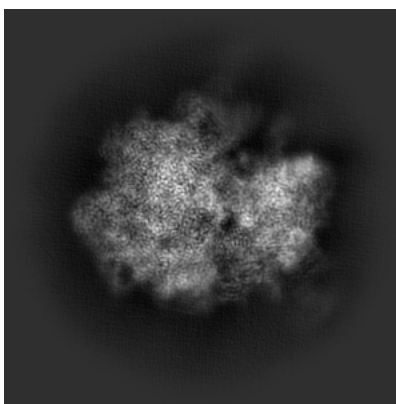
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

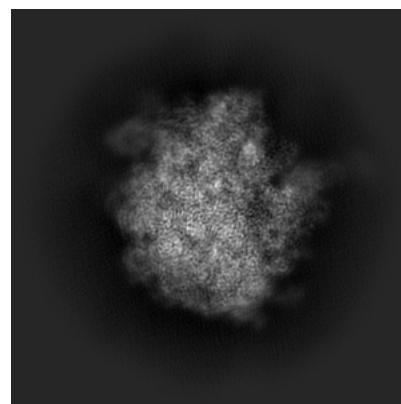
6.1.1 Primary map



X

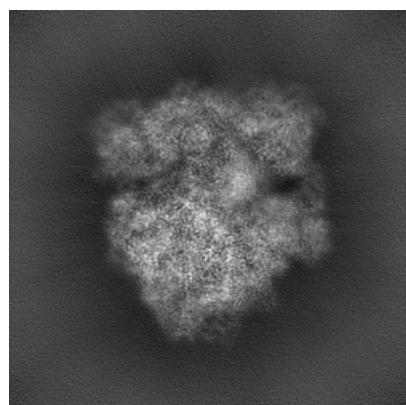


Y

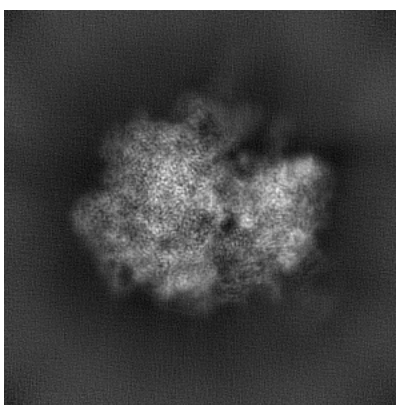


Z

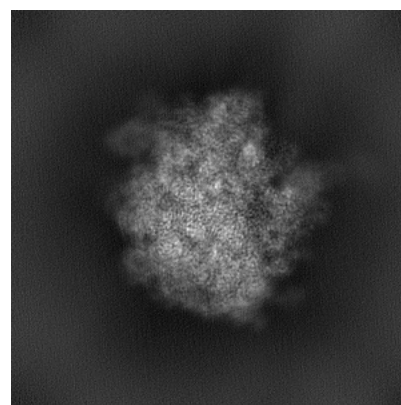
6.1.2 Raw map



X



Y

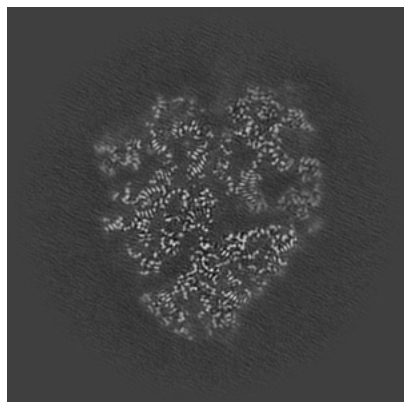


Z

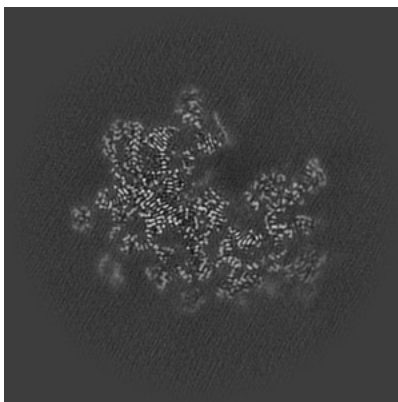
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

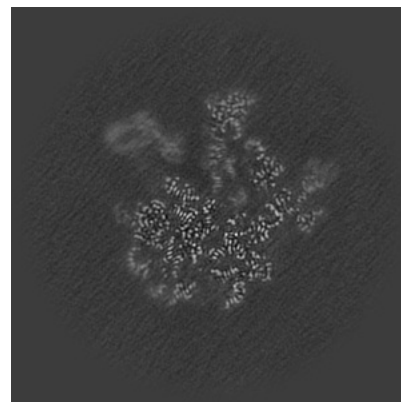
6.2.1 Primary map



X Index: 256

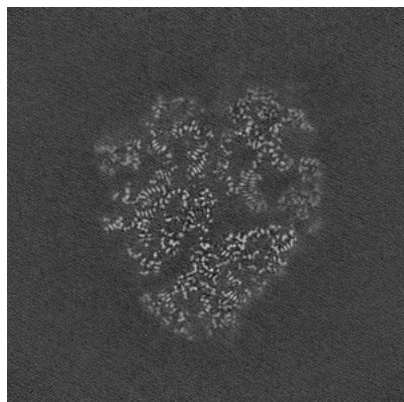


Y Index: 256

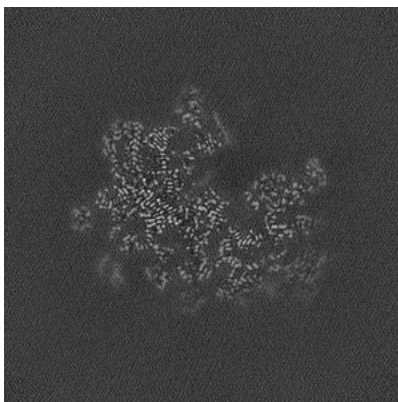


Z Index: 256

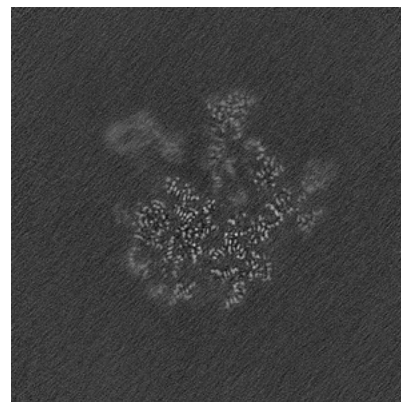
6.2.2 Raw map



X Index: 256



Y Index: 256

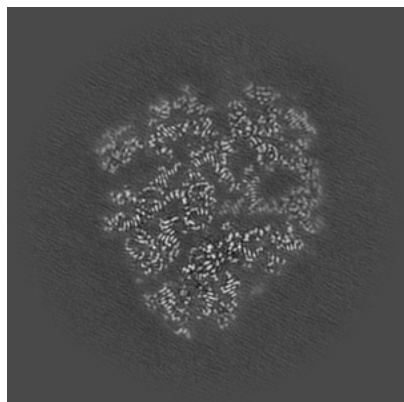


Z Index: 256

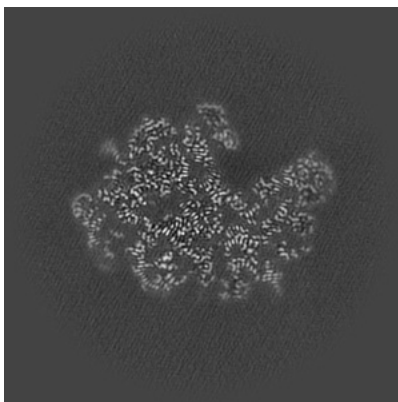
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

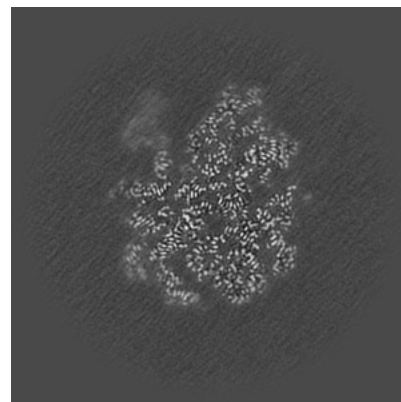
6.3.1 Primary map



X Index: 261

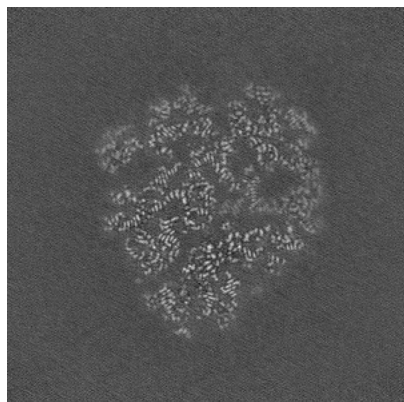


Y Index: 233

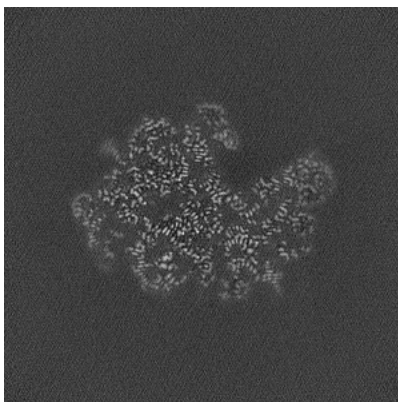


Z Index: 214

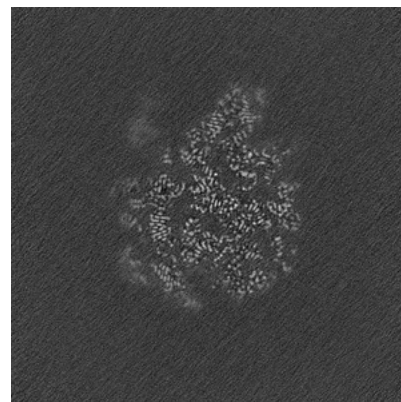
6.3.2 Raw map



X Index: 261



Y Index: 233

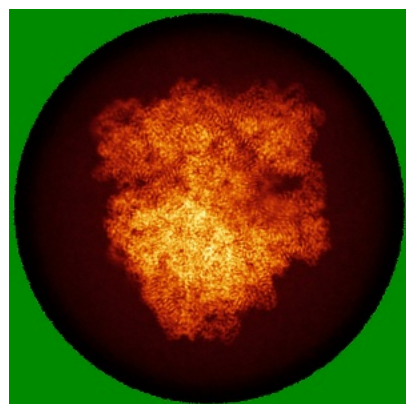


Z Index: 205

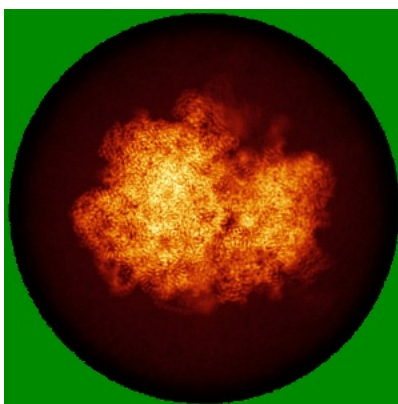
The images above show the largest variance slices of the map in three orthogonal directions.

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

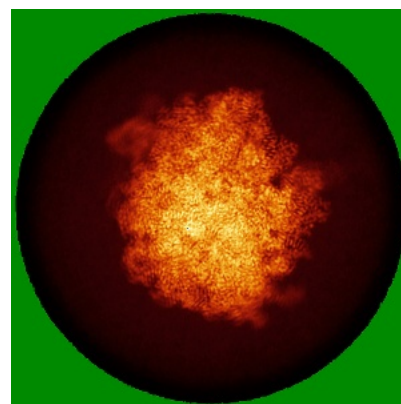
6.4.1 Primary map



X

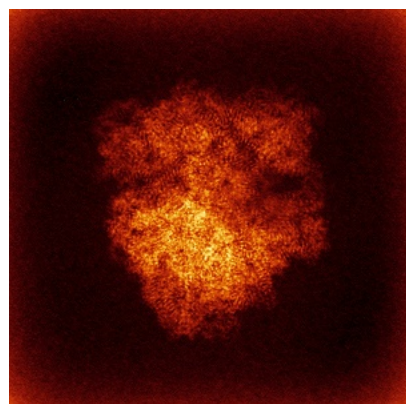


Y

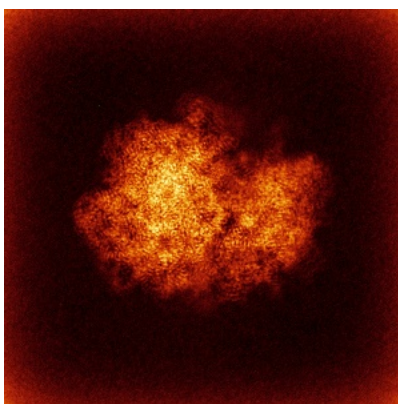


Z

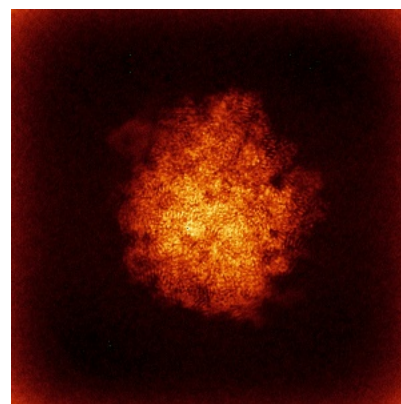
6.4.2 Raw map



X



Y

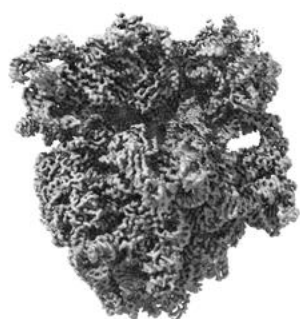


Z

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



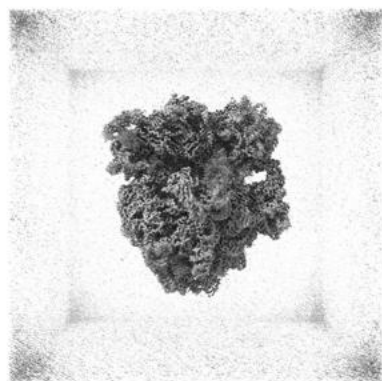
Y



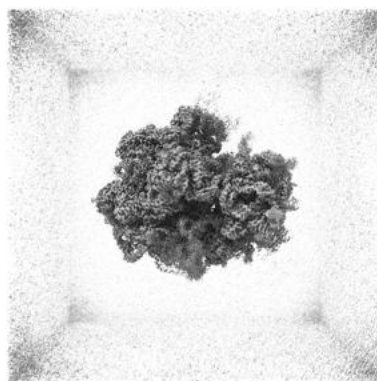
Z

The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

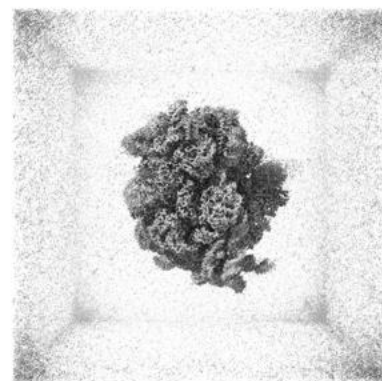
6.5.2 Raw map



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.

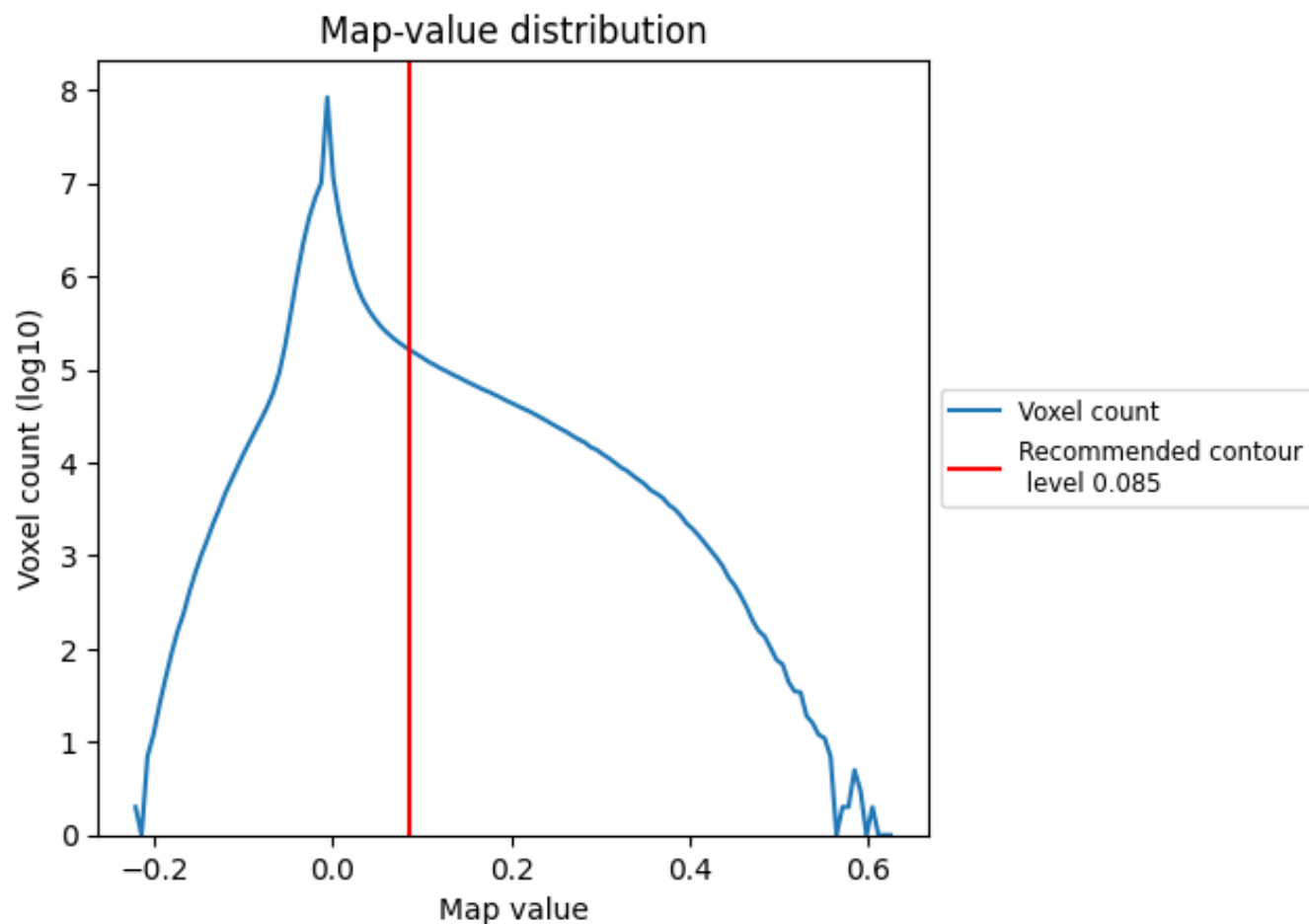
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

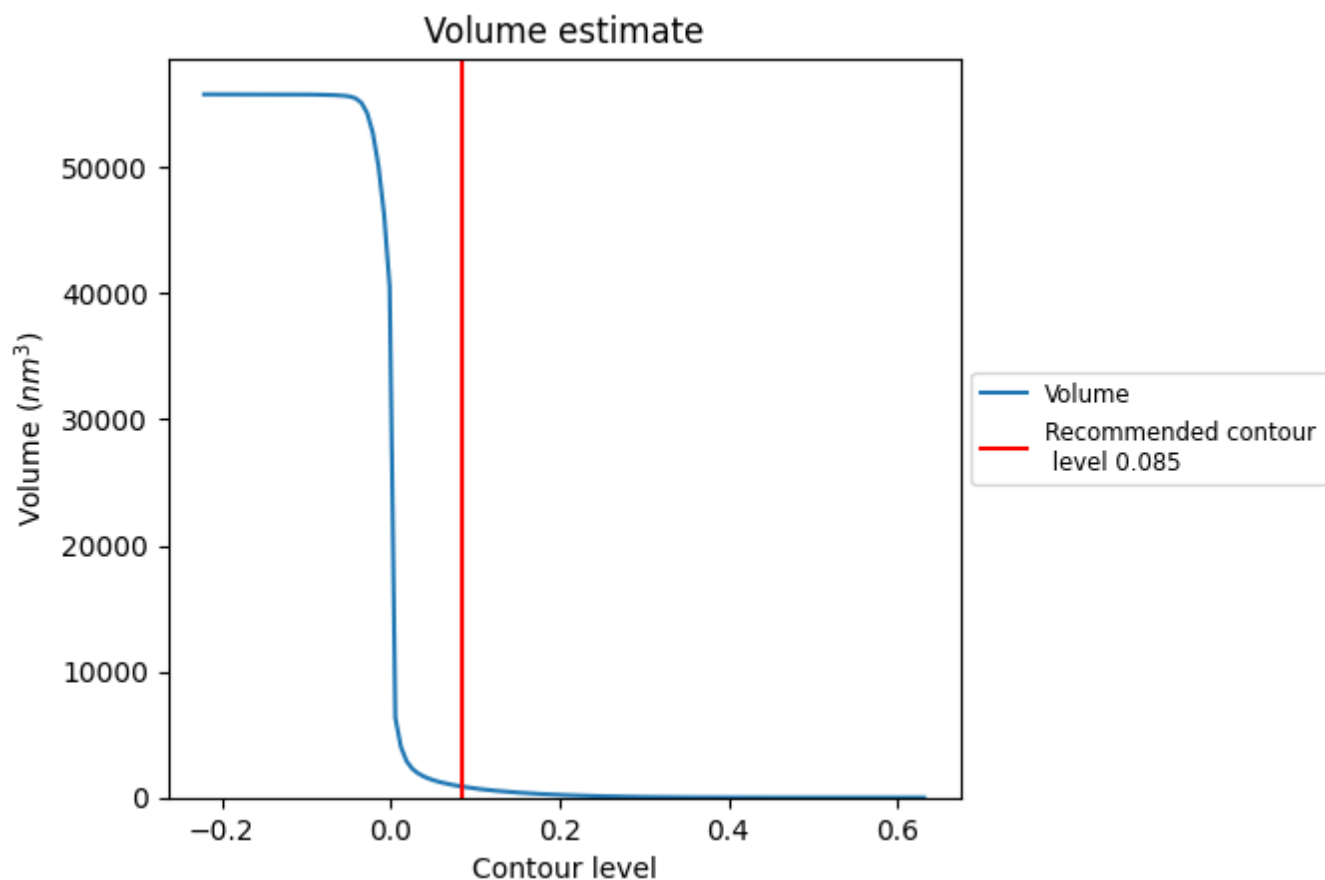
This section contains the results of statistical analysis of the map.

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.

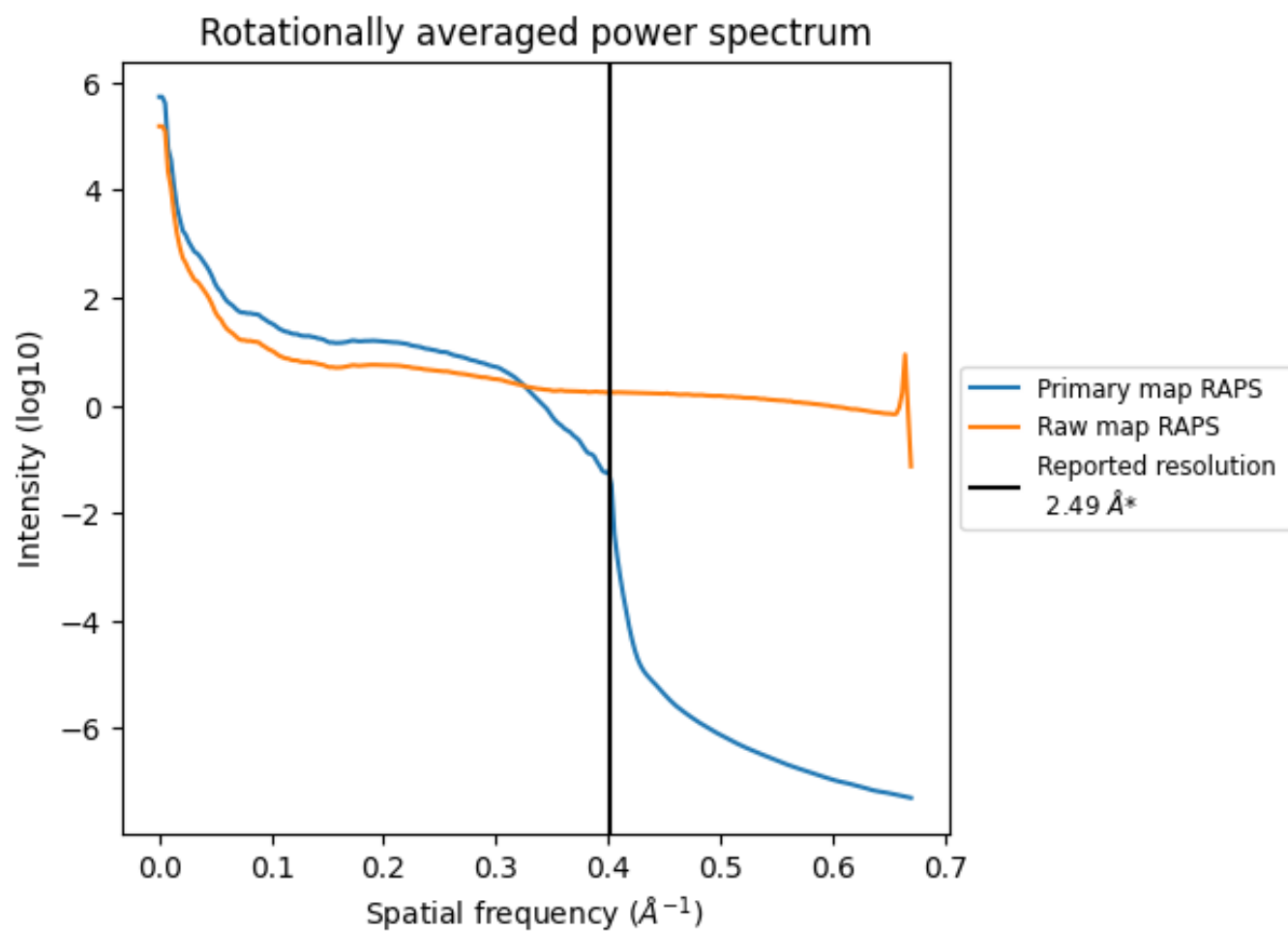
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 867 nm³; this corresponds to an approximate mass of 783 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

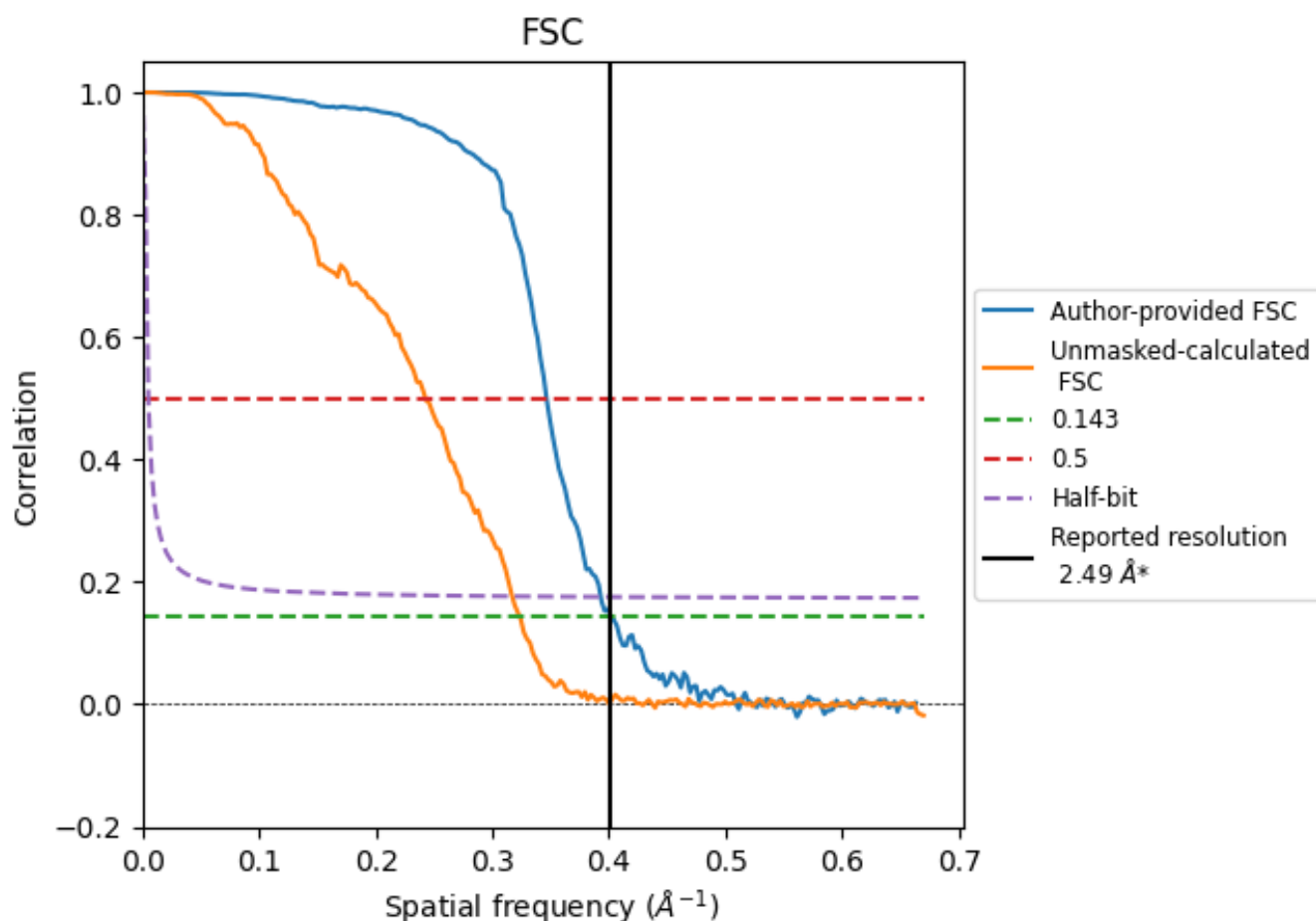


*Reported resolution corresponds to spatial frequency of 0.402 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.402 \AA^{-1}

8.2 Resolution estimates [i](#)

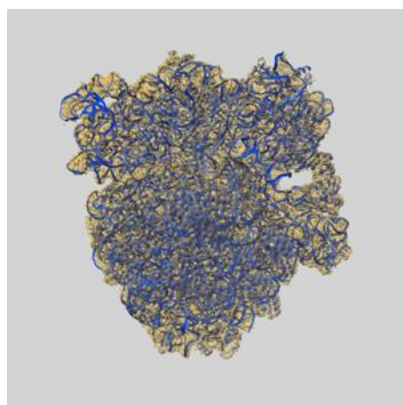
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.49	-	-
Author-provided FSC curve	2.49	2.89	2.54
Unmasked-calculated*	3.09	4.12	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.49 by more than 10 %

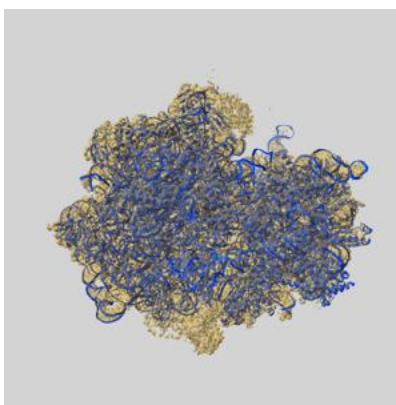
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51758 and PDB model 9H0L. Per-residue inclusion information can be found in section [3](#) on page [17](#).

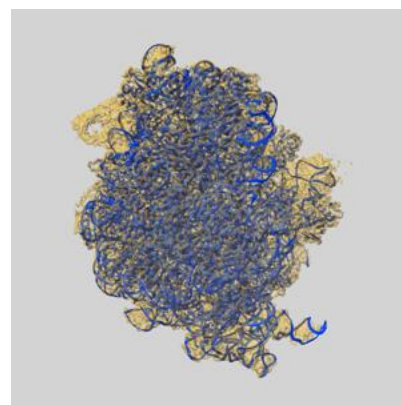
9.1 Map-model overlay [i](#)



X



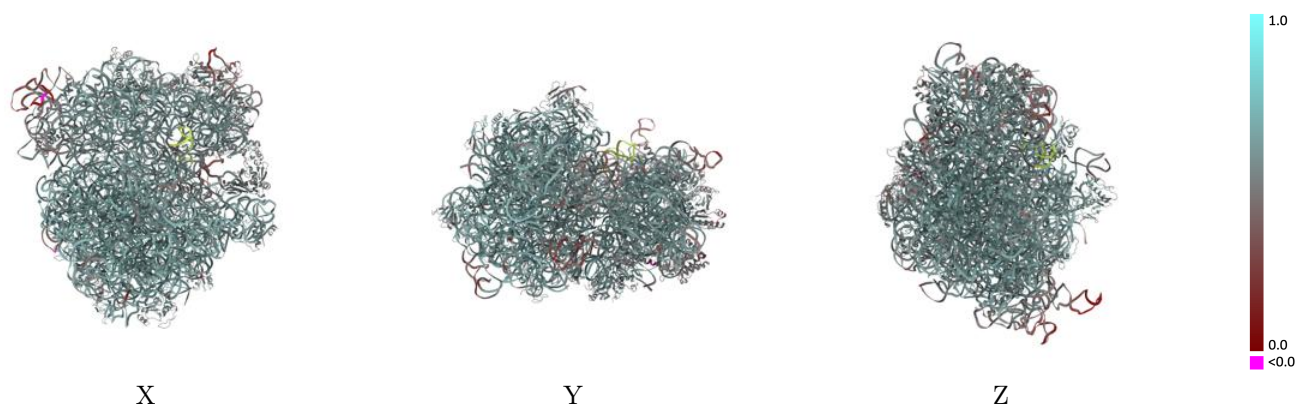
Y



Z

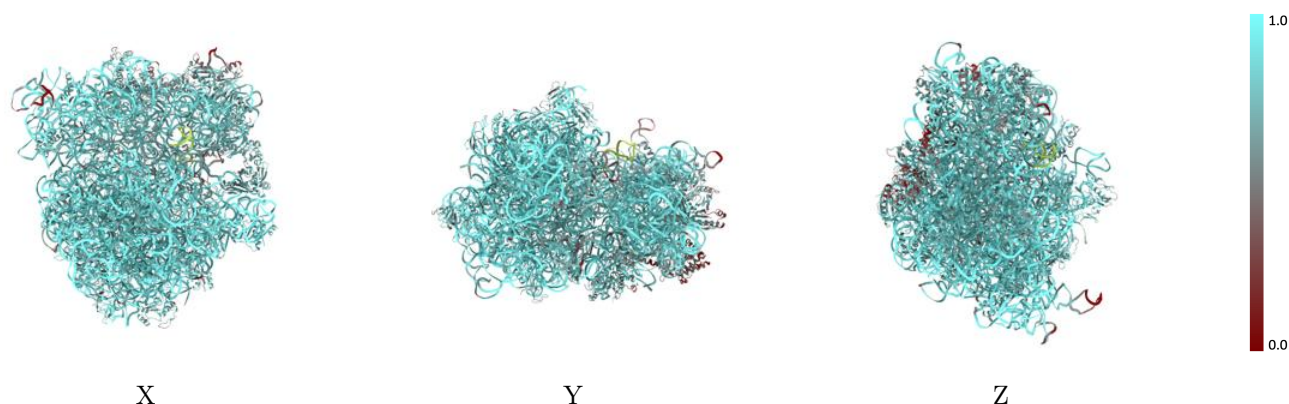
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



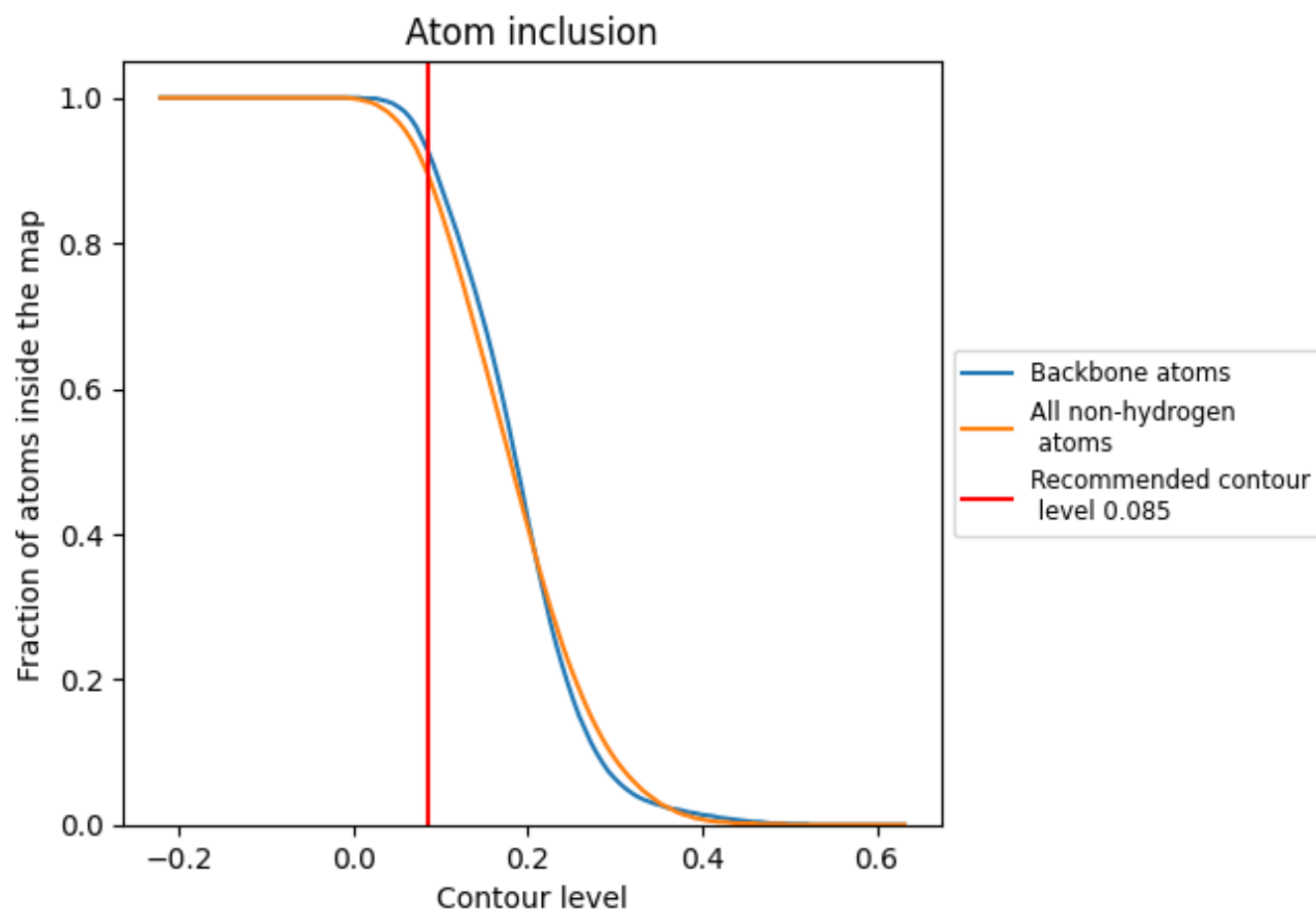
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.5860
0	 0.7750	 0.5880
1	 0.9380	 0.6420
2	 0.9210	 0.6380
3	 0.8770	 0.6040
4	 0.6800	 0.4760
A	 0.9360	 0.5790
B	 0.4040	 0.4590
C	 0.7430	 0.5510
D	 0.7080	 0.5310
E	 0.7920	 0.5850
F	 0.7310	 0.5240
G	 0.6760	 0.5240
H	 0.8260	 0.5730
I	 0.7700	 0.5330
J	 0.5860	 0.4810
K	 0.7820	 0.5720
L	 0.8150	 0.5980
M	 0.7420	 0.5350
N	 0.7600	 0.5520
O	 0.8000	 0.5530
P	 0.8290	 0.5650
Q	 0.7900	 0.5620
R	 0.7300	 0.5340
S	 0.7330	 0.5340
T	 0.7540	 0.5230
U	 0.5530	 0.4770
V	 0.5940	 0.3880
X	 0.9330	 0.6040
Y	 0.7380	 0.4900
Z	 0.8240	 0.5500
a	 0.9670	 0.6150
b	 0.9570	 0.5870
c	 0.9030	 0.6230
d	 0.8870	 0.6120



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Chain	Atom inclusion	Q-score
e	 0.8220	 0.5780
f	 0.7300	 0.5110
g	 0.7500	 0.5250
h	 0.6670	 0.5220
i	 0.8870	 0.6080
j	 0.8250	 0.6090
k	 0.8690	 0.6010
l	 0.8650	 0.6090
m	 0.9140	 0.6210
n	 0.8310	 0.5620
o	 0.8120	 0.5910
p	 0.9230	 0.6270
q	 0.8460	 0.6000
r	 0.8420	 0.6000
s	 0.8070	 0.5610
t	 0.7670	 0.5490
u	 0.8170	 0.5680
v	 0.8260	 0.6050
w	 0.8690	 0.6110
x	 0.7520	 0.5290
y	 0.8540	 0.5950
z	 0.8560	 0.6020