



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 05:28 PM JST

PDB ID : 8ZTU / pdb_00008ztu
EMDB ID : EMD-60473
Title : 70S ribosome arrested by PepNL
Authors : Ando, Y.; Kobo, A.; Nureki, O.; Taguchi, H.; Itoh, Y.; Chadani, Y.
Deposited on : 2024-06-07
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

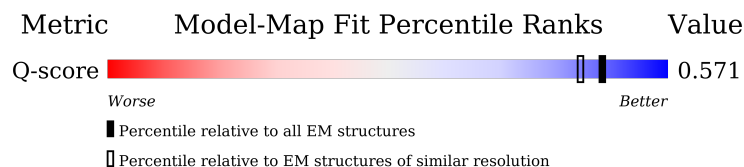
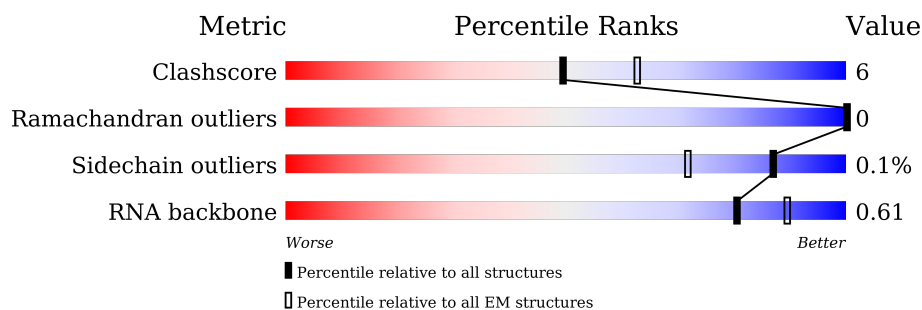
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	

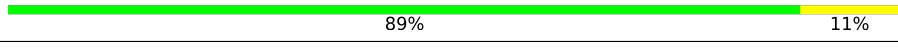
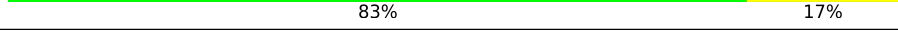
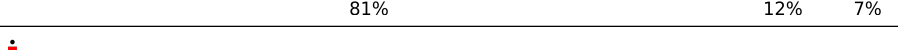
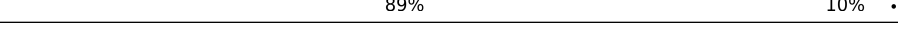
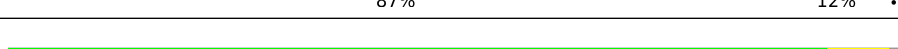
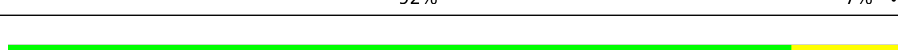
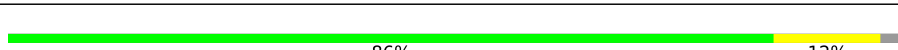
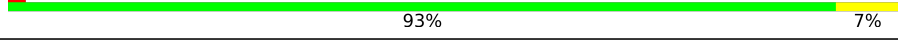
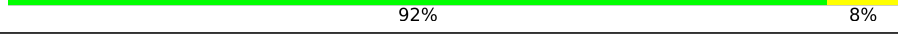
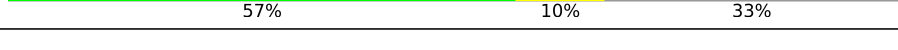
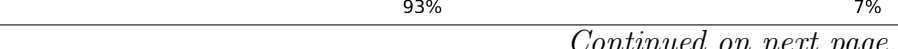
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Mol	Chain	Length	Quality of chain
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	

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Mol	Chain	Length	Quality of chain
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
46	y	59	
47	z	57	
48	0	55	
49	1	46	
50	2	65	
51	3	38	
52	4	70	
53	W	14	

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Mol	Chain	Length	Quality of chain
54	X	9	33% 89% 11%
55	Y	77	51% 36% 8% 5%
56	Z	3	67% 33%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 140242 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	1507	Total	C	N	O	P	0	0
			32360	14439	5944	10470	1507		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	225	Total	C	N	O	S	0	0
			1758	1112	316	322	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

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 30S ribosomal protein S4.

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 30S ribosomal protein S5.

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 30S ribosomal protein S6, 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 30S ribosomal protein S7.

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 30S ribosomal protein S8.

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 30S ribosomal protein S9.

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 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

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 30S ribosomal protein S12.

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 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

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 30S ribosomal protein S15.

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 30S ribosomal protein S16.

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 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

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 30S ribosomal protein S19.

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 30S ribosomal protein S20.

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 30S ribosomal protein S21.

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 23S rRNA.

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

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	67	Total	C	N	O	S	0	0
			505	322	90	92	1		

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	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
1	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called 50S ribosomal protein L17.

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

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	51	Total	C	N	O		0	0
			417	269	76	72			

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 53 is a protein called PepNL.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	W	14	Total	C	N	O	S	0	0
			108	70	17	20	1		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	X	9	Total	C	N	O	P	0	0
			194	87	37	61	9		

- Molecule 55 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Y	73	Total	C	N	O	P	0	0
			1563	695	281	514	73		

- Molecule 56 is a RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Z	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

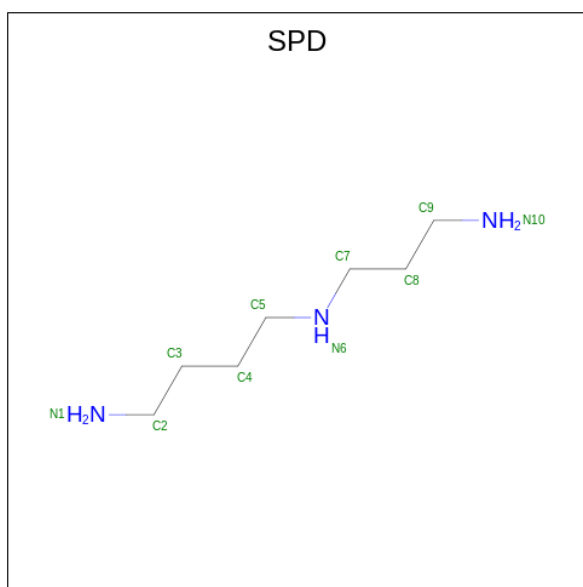
- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	83	Total	Mg	0
			83	83	
57	a	209	Total	Mg	0
			209	209	
57	b	5	Total	Mg	0
			5	5	
57	p	2	Total	Mg	0
			2	2	
57	z	1	Total	Mg	0
			1	1	

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

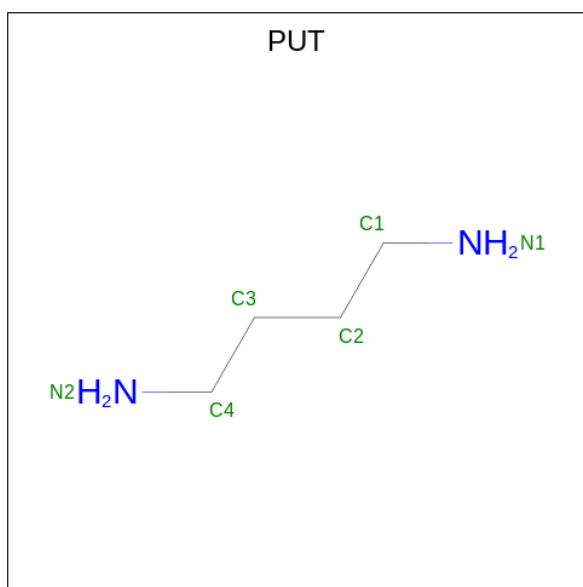
Mol	Chain	Residues	Atoms		AltConf
58	A	4	Total	K	0
			4	4	
58	D	1	Total	K	0
			1	1	
58	a	40	Total	K	0
			40	40	
58	c	2	Total	K	0
			2	2	

- Molecule 59 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



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

- Molecule 60 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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

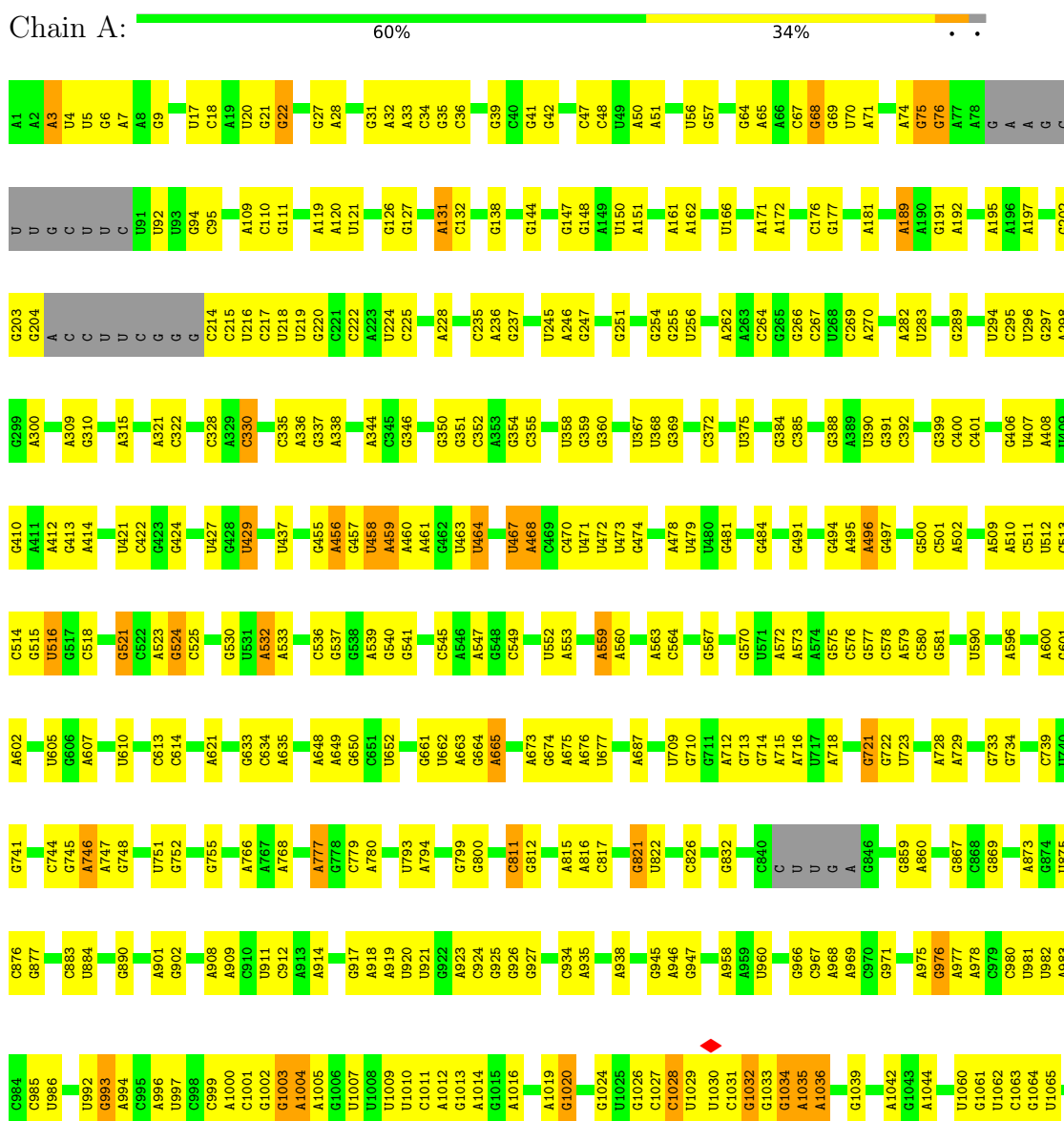
- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

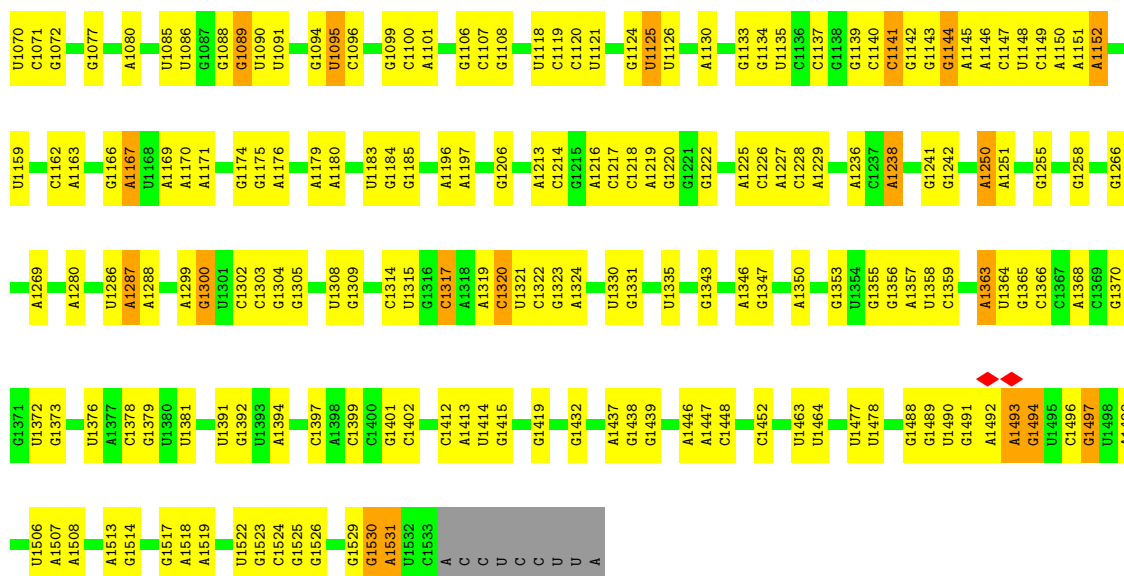
Mol	Chain	Residues	Atoms		AltConf
61	3	1	Total	Zn	0
			1	1	
61	4	1	Total	Zn	0
			1	1	

3 Residue-property plots

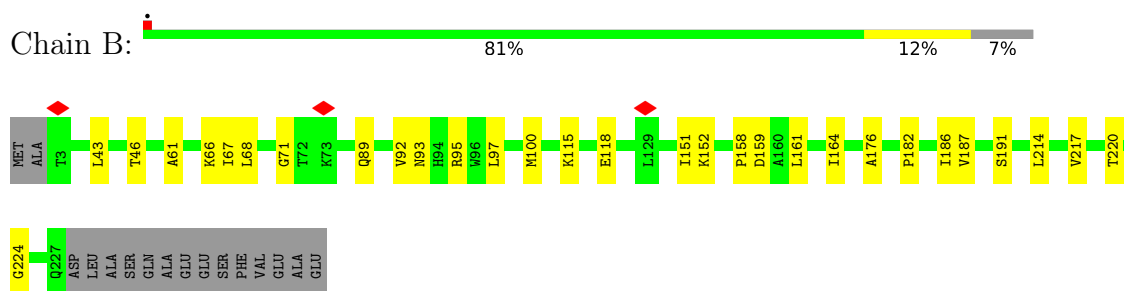
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

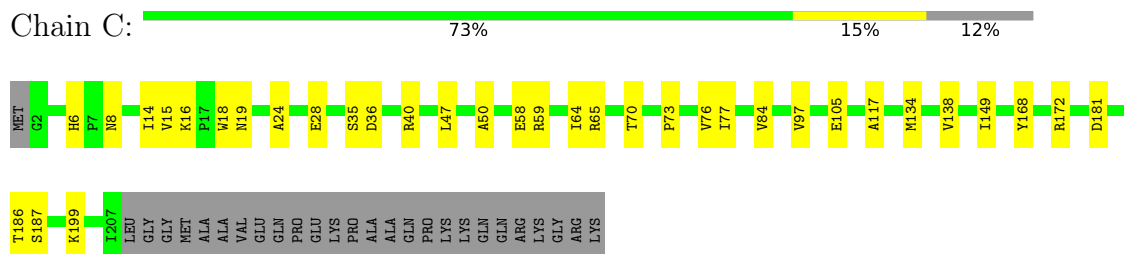




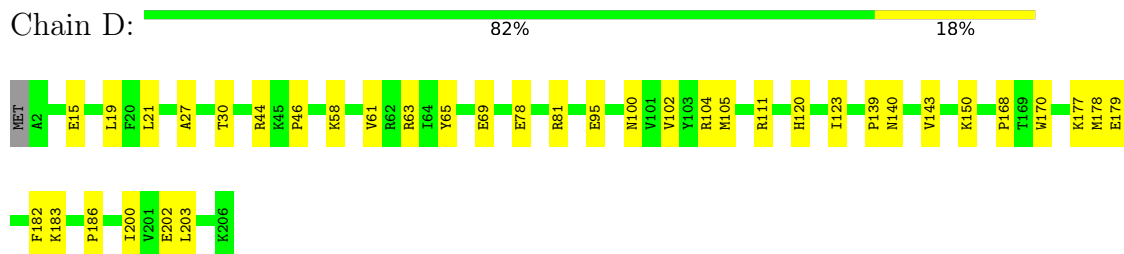
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



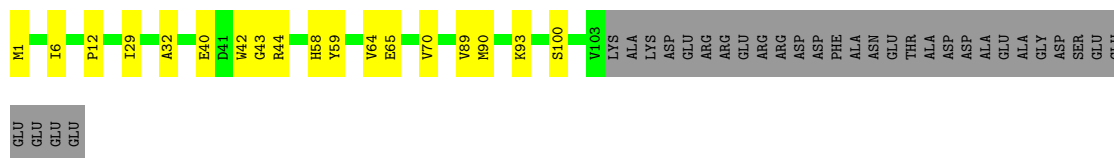
• Molecule 5: 30S ribosomal protein S5

Chain E:  84% 9% 7%



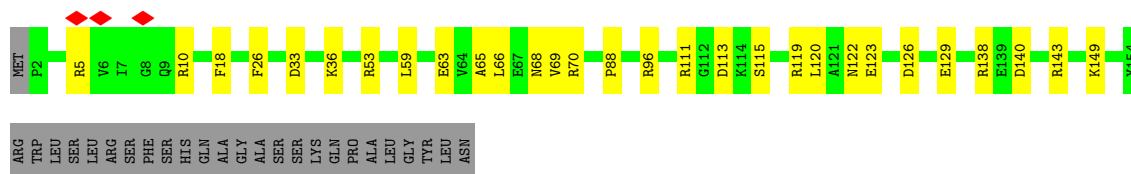
- Molecule 6: 30S ribosomal protein S6, fully modified isoform

Chain F:  63% 13% 24%



- Molecule 7: 30S ribosomal protein S7

Chain G:  69% 16% 15%



- Molecule 8: 30S ribosomal protein S8

Chain H:  92% 7%



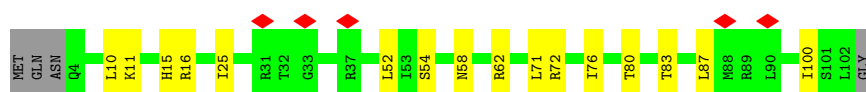
- Molecule 9: 30S ribosomal protein S9

Chain I:  78% 20%



- Molecule 10: 30S ribosomal protein S10

Chain J:  5% 81% 16%

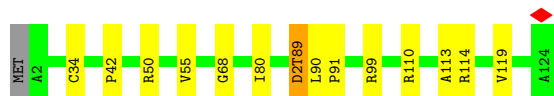
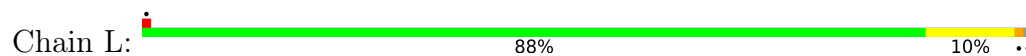


- Molecule 11: 30S ribosomal protein S11

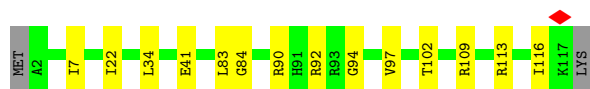
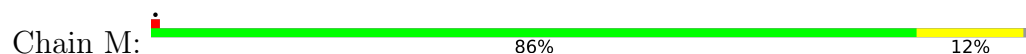
Chain K:  74% 17% 9%



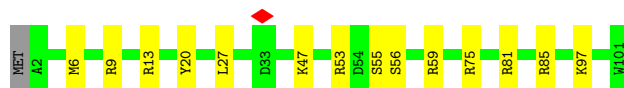
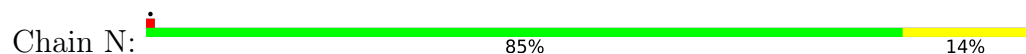
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



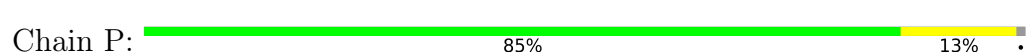
- Molecule 14: 30S ribosomal protein S14



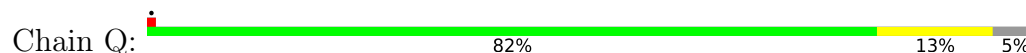
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

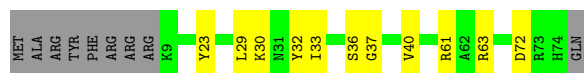


- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

Chain R:  73% 15% 12%



- Molecule 19: 30S ribosomal protein S19

Chain S:  85% 7% 9%



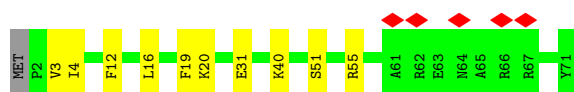
- Molecule 20: 30S ribosomal protein S20

Chain T:  82% 17% .



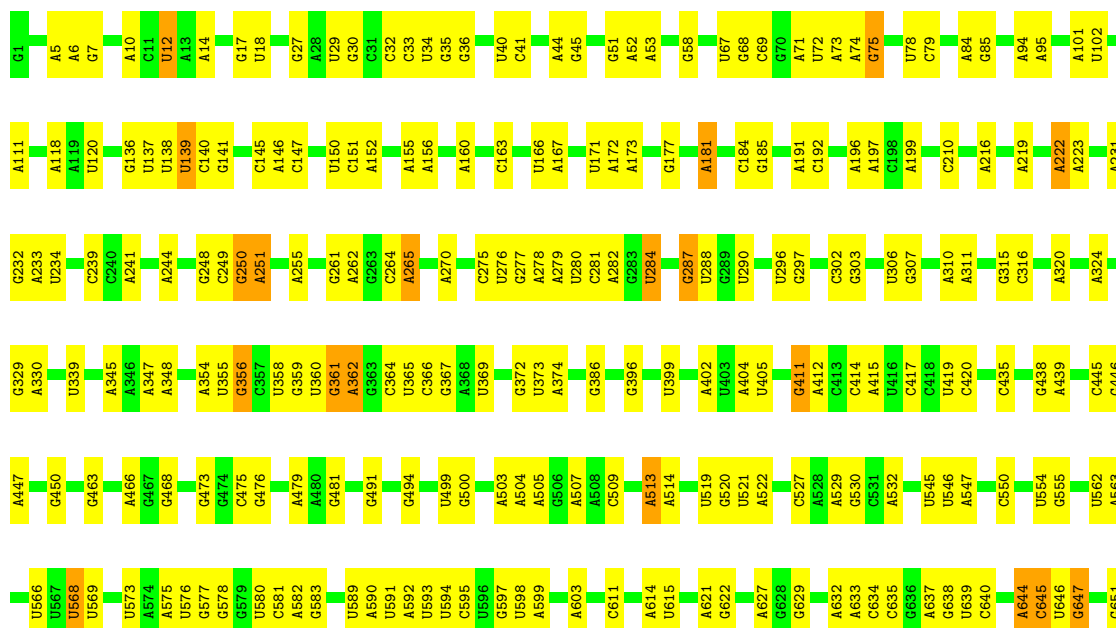
- Molecule 21: 30S ribosomal protein S21

Chain U:  7% 85% 14% .

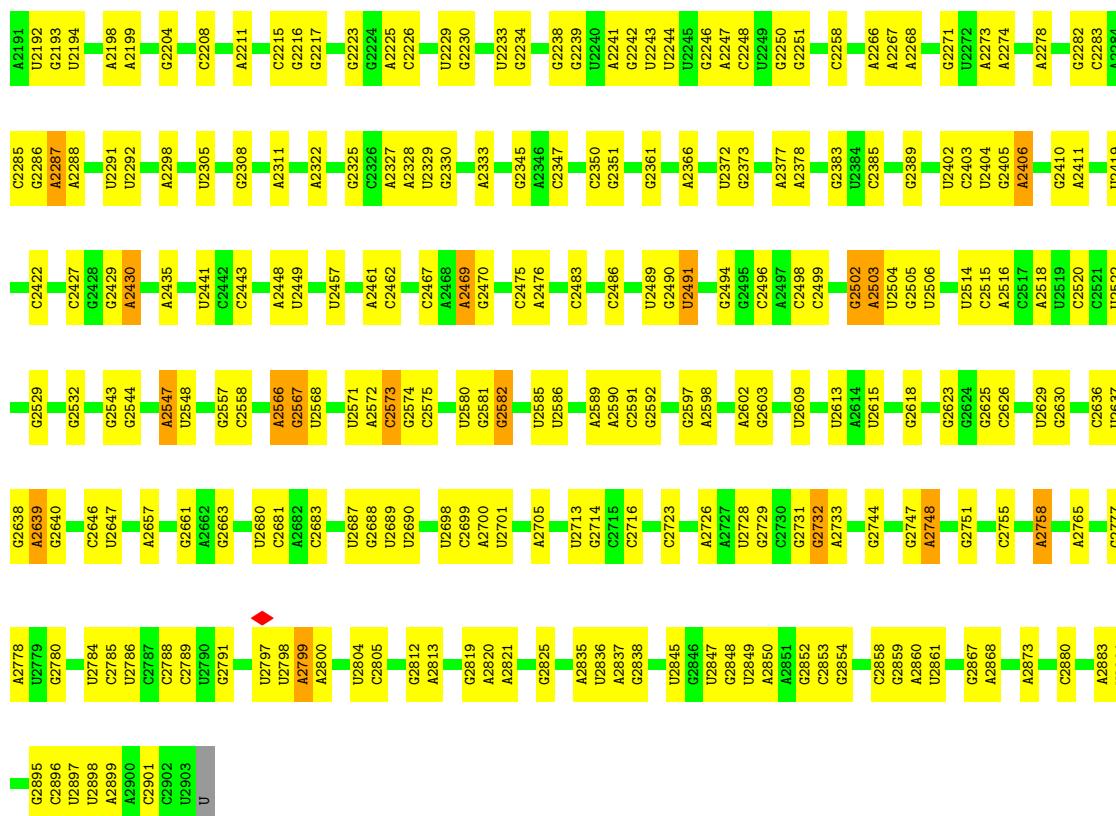


- Molecule 22: 23S rRNA

Chain a:  61% 31% . 5%



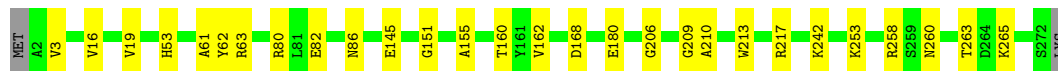
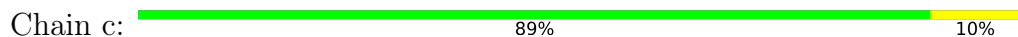




• Molecule 23: 5S rRNA



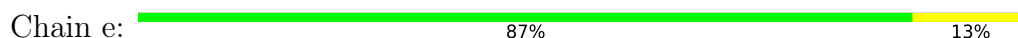
• Molecule 24: 50S ribosomal protein L2



• Molecule 25: 50S ribosomal protein L3

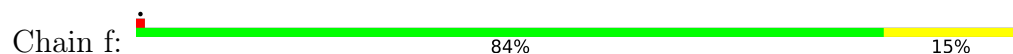


• Molecule 26: 50S ribosomal protein L4

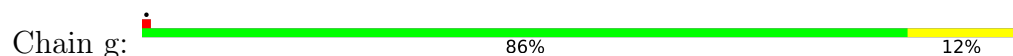




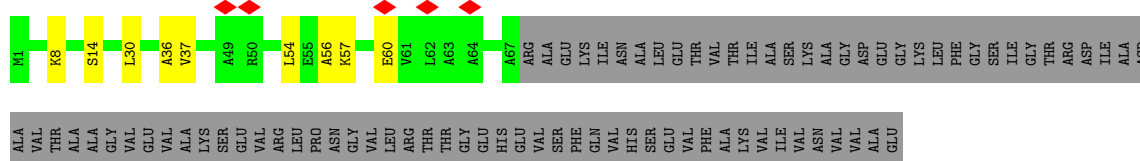
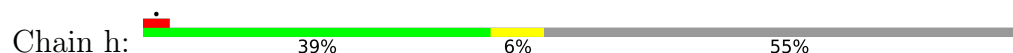
- Molecule 27: 50S ribosomal protein L5



- Molecule 28: 50S ribosomal protein L6



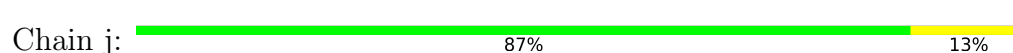
- Molecule 29: 50S ribosomal protein L9



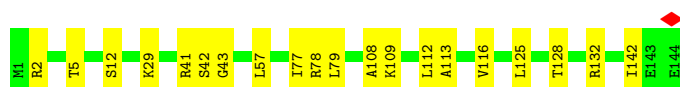
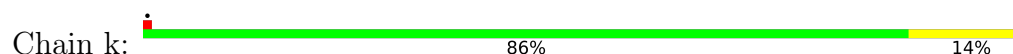
- Molecule 30: 50S ribosomal protein L13



- Molecule 31: 50S ribosomal protein L14



- Molecule 32: 50S ribosomal protein L15



- Molecule 33: 50S ribosomal protein L16

Chain l:  83% 17%



- Molecule 34: 50S ribosomal protein L17

Chain m:  81% 12% 7%



- Molecule 35: 50S ribosomal protein L18

Chain n:  89% 10%



- Molecule 36: 50S ribosomal protein L19

Chain o:  87% 12%



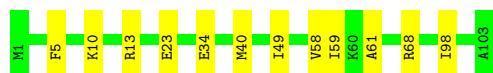
- Molecule 37: 50S ribosomal protein L20

Chain p:  92% 7%



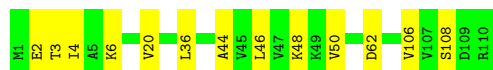
- Molecule 38: 50S ribosomal protein L21

Chain q:  88% 12%



- Molecule 39: 50S ribosomal protein L22

Chain r:  88% 12%



- Molecule 40: 50S ribosomal protein L23

Chain s:  87% 6% 7%



- Molecule 41: 50S ribosomal protein L24

Chain t:  86% 12% 2%



- Molecule 42: 50S ribosomal protein L25

Chain u:  67% 33% 0%



- Molecule 43: 50S ribosomal protein L27

Chain v:  81% 11% 8%



- Molecule 44: 50S ribosomal protein L28

Chain w:  81% 18% 1%



- Molecule 45: 50S ribosomal protein L29

Chain x:  89% 10% 1%



- Molecule 46: 50S ribosomal protein L30

Chain y:  85% 14% 1%



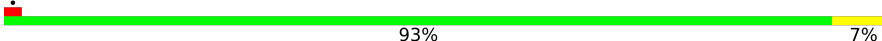
• Molecule 47: 50S ribosomal protein L32

Chain z:  89% 9% .

• Molecule 48: 50S ribosomal protein L33

Chain 0:  73% 20% 7%

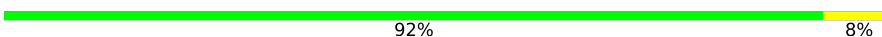
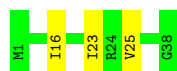
• Molecule 49: 50S ribosomal protein L34

Chain 1:  93% 7%

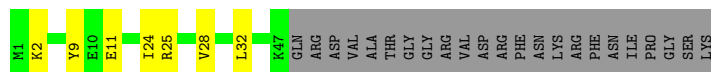
• Molecule 50: 50S ribosomal protein L35

Chain 2:  83% 15% .

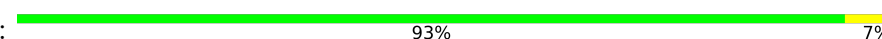
• Molecule 51: 50S ribosomal protein L36

Chain 3:  92% 8%

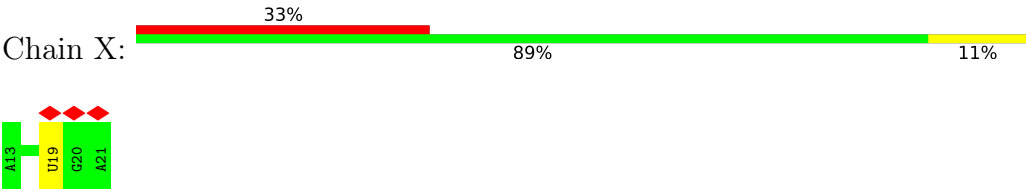
• Molecule 52: 50S ribosomal protein L31

Chain 4:  57% 10% 33%

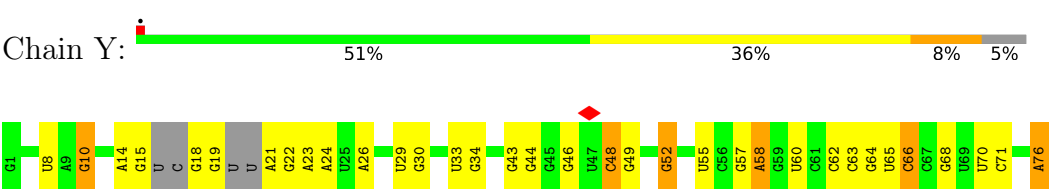
• Molecule 53: PepNL

Chain W:  93% 7%

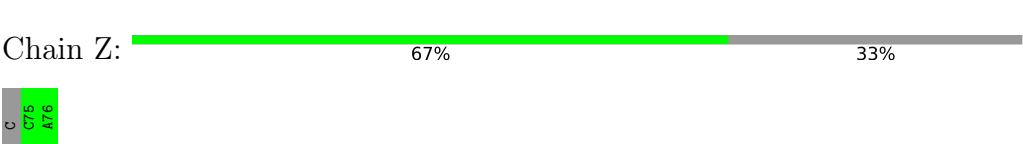
● Molecule 54: mRNA



● Molecule 55: P-tRNA



● Molecule 56: E-tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87514	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.050	Depositor
Minimum map value	-0.688	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	358.56, 358.56, 358.56	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.10	0/35954	0.22	0/56077
2	B	0.09	0/1789	0.23	0/2410
3	C	0.09	0/1651	0.23	0/2225
4	D	0.09	0/1665	0.22	0/2227
5	E	0.09	0/1165	0.23	0/1568
6	F	0.10	0/858	0.26	0/1160
7	G	0.13	0/1219	0.25	0/1635
8	H	0.08	0/989	0.23	0/1326
9	I	0.09	0/1034	0.23	0/1375
10	J	0.10	0/805	0.29	0/1089
11	K	0.12	0/884	0.23	0/1191
12	L	0.09	0/960	0.23	0/1286
13	M	0.09	0/909	0.23	0/1215
14	N	0.08	0/817	0.19	0/1088
15	O	0.07	0/722	0.18	0/964
16	P	0.09	0/653	0.25	0/877
17	Q	0.09	0/657	0.26	0/881
18	R	0.11	0/553	0.24	0/742
19	S	0.08	0/685	0.19	0/922
20	T	0.12	0/676	0.23	0/895
21	U	0.08	0/597	0.20	0/792
22	a	0.10	0/65651	0.23	0/102413
23	b	0.08	0/2850	0.21	0/4444
24	c	0.10	0/2121	0.25	0/2852
25	d	0.09	0/1576	0.23	0/2119
26	e	0.09	0/1571	0.23	0/2113
27	f	0.10	0/1434	0.26	0/1926
28	g	0.08	0/1324	0.23	0/1794
29	h	0.12	0/510	0.29	0/687
30	i	0.09	0/1152	0.22	0/1551
31	j	0.10	0/955	0.25	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	k	0.09	0/1062	0.23	0/1413
33	l	0.10	0/1073	0.24	0/1433
34	m	0.11	0/958	0.27	0/1281
35	n	0.09	0/902	0.23	0/1209
36	o	0.11	0/929	0.25	0/1242
37	p	0.10	0/960	0.24	0/1278
38	q	0.10	0/829	0.27	0/1107
39	r	0.09	0/864	0.25	0/1156
40	s	0.08	0/744	0.21	0/994
41	t	0.08	0/787	0.22	0/1051
42	u	0.10	0/766	0.26	0/1025
43	v	0.09	0/599	0.24	0/792
44	w	0.10	0/635	0.25	0/848
45	x	0.08	0/502	0.17	0/667
46	y	0.09	0/453	0.23	0/605
47	z	0.19	0/450	0.26	0/599
48	0	0.09	0/424	0.22	0/565
49	1	0.10	0/380	0.31	0/498
50	2	0.10	0/513	0.25	0/676
51	3	0.09	0/303	0.22	0/397
52	4	0.07	0/371	0.22	0/496
53	W	0.24	0/99	0.62	0/133
54	X	0.08	0/217	0.23	0/336
55	Y	0.12	0/1744	0.25	0/2714
56	Z	0.07	0/46	0.13	0/69
All	All	0.10	0/150996	0.23	0/225707

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32360	0	16304	347	0
2	B	1758	0	1782	17	0
3	C	1624	0	1696	19	0
4	D	1643	0	1707	21	0
5	E	1152	0	1196	11	0
6	F	839	0	833	10	0
7	G	1203	0	1254	20	0
8	H	979	0	1031	8	0
9	I	1022	0	1070	18	0
10	J	795	0	836	12	0
11	K	877	0	884	15	0
12	L	957	0	1017	13	0
13	M	900	0	965	9	0
14	N	805	0	844	14	0
15	O	714	0	734	5	0
16	P	643	0	661	7	0
17	Q	648	0	691	9	0
18	R	544	0	565	6	0
19	S	668	0	693	4	0
20	T	670	0	719	9	0
21	U	589	0	629	6	0
22	a	59130	0	29763	550	0
23	b	2549	0	1291	22	0
24	c	2082	0	2154	18	0
25	d	1566	0	1617	13	0
26	e	1552	0	1619	18	0
27	f	1410	0	1444	16	0
28	g	1304	0	1345	16	0
29	h	505	0	532	4	0
30	i	1129	0	1162	10	0
31	j	946	0	1023	11	0
32	k	1053	0	1129	14	0
33	l	1075	0	1145	15	0
34	m	945	0	989	8	0
35	n	892	0	923	7	0
36	o	917	0	962	11	0
37	p	947	0	1019	6	0
38	q	816	0	839	7	0
39	r	857	0	922	7	0
40	s	738	0	807	4	0
41	t	779	0	831	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	u	753	0	780	20	0
43	v	592	0	607	6	0
44	w	625	0	652	9	0
45	x	501	0	531	4	0
46	y	449	0	488	4	0
47	z	444	0	458	3	0
48	0	417	0	451	7	0
49	1	377	0	418	3	0
50	2	504	0	572	7	0
51	3	302	0	340	2	0
52	4	364	0	362	5	0
53	W	108	0	112	1	0
54	X	194	0	98	0	0
55	Y	1563	0	791	22	0
56	Z	42	0	23	0	0
57	A	83	0	0	0	0
57	a	209	0	0	0	0
57	b	5	0	0	0	0
57	p	2	0	0	0	0
57	z	1	0	0	0	0
58	A	4	0	0	0	0
58	D	1	0	0	0	0
58	a	40	0	0	0	0
58	c	2	0	0	0	0
59	a	70	0	133	7	0
60	a	6	0	12	0	0
61	3	1	0	0	0	0
61	4	1	0	0	0	0
All	All	140242	0	94455	1295	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1295) 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)
22:a:284:U:H3	22:a:356:G:H1	1.14	0.89
22:a:881:G:H1	22:a:895:U:H3	1.22	0.88
7:G:113:ASP:HB2	7:G:119:ARG:HG2	1.60	0.81
22:a:848:C:H2'	22:a:849:A:H8	1.49	0.76
1:A:111:G:H1	1:A:330:C:H41	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:G:N2	1:A:1125:U:O4	2.20	0.72
22:a:355:U:H2'	22:a:356:G:C8	2.25	0.72
22:a:320:A:N3	26:e:163:ASN:ND2	2.37	0.72
1:A:1149:C:H2'	1:A:1150:A:H8	1.55	0.71
1:A:744:C:H2'	1:A:745:G:H8	1.55	0.70
18:R:30:LYS:HA	18:R:33:ILE:HG12	1.73	0.70
1:A:521:G:HO2'	1:A:536:C:HO2'	1.40	0.69
27:f:102:ARG:HG2	52:4:24:ILE:HD12	1.75	0.68
22:a:197:A:N6	22:a:2430:A:O2'	2.26	0.68
7:G:113:ASP:H	7:G:119:ARG:HD3	1.59	0.68
1:A:673:A:H2'	1:A:674:G:C8	2.28	0.68
27:f:58:ALA:HB2	27:f:65:PRO:HD3	1.77	0.67
32:k:108:ALA:HB3	32:k:125:LEU:HD22	1.75	0.67
22:a:2848:G:O2'	22:a:2867:G:N2	2.28	0.67
23:b:30:C:H1'	23:b:57:A:H61	1.59	0.67
55:Y:18:G:O2'	55:Y:57:G:N2	2.28	0.67
22:a:270:A:N1	22:a:369:U:O2'	2.24	0.66
24:c:53:HIS:HA	24:c:217:ARG:HB2	1.77	0.66
1:A:1026:G:H1	1:A:1035:A:N6	1.94	0.66
22:a:820:A:H4'	22:a:836:G:H22	1.60	0.66
22:a:1724:G:O6	22:a:1737:G:N2	2.29	0.66
1:A:826:C:O2	8:H:16:ASN:ND2	2.29	0.65
1:A:1086:U:H3	1:A:1099:G:H22	1.42	0.65
22:a:1779:U:OP2	22:a:1784:A:N6	2.24	0.65
33:l:50:ARG:HA	33:l:53:MET:HE2	1.77	0.65
22:a:210:C:OP1	49:1:29:GLN:NE2	2.29	0.65
22:a:475:C:O2	22:a:479:A:N6	2.27	0.65
22:a:2728:U:HO2'	22:a:2729:G:H8	1.45	0.65
1:A:1376:U:O4	7:G:10:ARG:NH1	2.30	0.65
27:f:49:LEU:HD22	27:f:148:ARG:HH12	1.62	0.65
1:A:713:G:H2'	1:A:714:G:C8	2.32	0.64
22:a:651:G:H5'	50:2:19:LYS:HB2	1.80	0.64
1:A:219:U:H2'	1:A:220:G:H8	1.61	0.64
22:a:1722:A:N6	22:a:1738:G:O2'	2.31	0.64
1:A:946:A:H2'	1:A:947:G:C8	2.33	0.64
22:a:856:G:H2'	22:a:857:G:C8	2.33	0.63
5:E:115:LEU:HD13	5:E:123:VAL:HG11	1.80	0.63
22:a:1311:G:OP2	22:a:1311:G:N2	2.25	0.63
23:b:77:U:OP1	42:u:21:ARG:NH1	2.30	0.63
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.81	0.63
1:A:18:C:OP1	5:E:132:ASN:ND2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:e:16:GLU:O	26:e:20:GLY:N	2.32	0.63
22:a:2483:C:N3	33:l:123:LYS:NZ	2.47	0.63
42:u:64:VAL:HG22	42:u:69:GLU:HG2	1.80	0.63
18:R:37:GLY:O	18:R:63:ARG:NH2	2.32	0.63
22:a:2246:G:H2'	22:a:2247:A:H8	1.64	0.63
30:i:96:ARG:HD2	30:i:99:ARG:HG3	1.80	0.63
1:A:662:U:OP2	6:F:93:LYS:NZ	2.30	0.62
1:A:718:A:O2'	21:U:31:GLU:OE2	2.16	0.62
33:l:77:PRO:HG2	33:l:80:VAL:HG21	1.81	0.62
55:Y:18:G:N2	55:Y:58:A:OP2	2.31	0.62
22:a:698:C:O2'	22:a:734:A:N6	2.32	0.62
1:A:1071:C:H2'	1:A:1072:G:H8	1.63	0.62
1:A:674:G:H2'	1:A:675:A:H8	1.64	0.62
22:a:1802:A:H2'	22:a:1803:A:C8	2.35	0.62
1:A:1397:C:OP2	5:E:29:ARG:NH2	2.32	0.62
5:E:165:LEU:O	8:H:114:ARG:NH1	2.32	0.62
22:a:976:G:HO2'	22:a:1155:A:HO2'	1.44	0.62
22:a:1386:C:H2'	22:a:1387:A:H8	1.64	0.62
1:A:1222:G:OP2	1:A:1322:C:N4	2.32	0.61
3:C:35:SER:OG	3:C:59:ARG:NH2	2.34	0.61
1:A:946:A:H2'	1:A:947:G:H8	1.65	0.61
28:g:164:TYR:HB2	28:g:167:GLU:HB2	1.82	0.61
22:a:581:C:H2'	22:a:582:A:H8	1.65	0.61
22:a:1129:A:N6	22:a:2491:U:OP1	2.32	0.61
31:j:9:ASN:OD1	31:j:18:ARG:NH1	2.33	0.61
22:a:1386:C:H2'	22:a:1387:A:C8	2.34	0.61
1:A:1266:G:N2	1:A:1269:A:OP2	2.26	0.61
1:A:1034:G:H2'	1:A:1035:A:H8	1.66	0.61
2:B:115:LYS:NZ	2:B:152:LYS:O	2.33	0.61
1:A:195:A:N3	1:A:222:C:O2'	2.33	0.60
1:A:875:U:O2'	8:H:15:ARG:NH1	2.33	0.60
6:F:29:ILE:HD13	6:F:64:VAL:HG11	1.82	0.60
22:a:160:A:N3	22:a:2208:C:O2'	2.33	0.60
1:A:1175:G:H2'	1:A:1176:A:H8	1.66	0.60
22:a:1417:C:HO2'	22:a:1587:G:HO2'	1.46	0.60
22:a:2246:G:H2'	22:a:2247:A:C8	2.36	0.60
1:A:501:C:H2'	1:A:502:A:H8	1.66	0.60
1:A:335:C:H2'	1:A:336:A:H8	1.65	0.60
1:A:664:G:H22	1:A:741:G:H1	1.48	0.60
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.83	0.60
38:q:10:LYS:NZ	38:q:23:GLU:OE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1032:A:H1'	51:3:23:ILE:HD13	1.84	0.59
1:A:980:C:O2'	14:N:13:ARG:NH1	2.36	0.59
22:a:500:G:N1	22:a:503:A:OP2	2.32	0.59
12:L:68:GLY:O	12:L:99:ARG:NH1	2.34	0.59
35:n:83:LEU:HD11	35:n:114:GLY:HA3	1.83	0.59
1:A:401:C:O2'	1:A:621:A:N3	2.30	0.59
47:z:43:ILE:HG22	47:z:49:TYR:HB2	1.84	0.59
22:a:75:G:H22	22:a:111:A:H2	1.51	0.59
1:A:75:G:H3'	1:A:76:G:H8	1.68	0.59
28:g:50:LEU:HD13	28:g:72:LEU:HD23	1.84	0.59
7:G:70:ARG:HG2	7:G:96:ARG:HB3	1.85	0.59
27:f:102:ARG:NH1	52:4:9:TYR:OH	2.36	0.59
1:A:375:U:O2	16:P:28:ARG:NH1	2.35	0.59
17:Q:19:LYS:H	17:Q:51:ASN:HD21	1.51	0.58
55:Y:15:G:H22	55:Y:48:C:H42	1.51	0.58
22:a:503:A:H4'	22:a:504:A:H3'	1.86	0.58
22:a:1252:G:H1	37:p:37:GLN:HE21	1.51	0.58
24:c:155:ALA:HB2	24:c:162:VAL:HG23	1.85	0.58
1:A:714:G:H2'	1:A:715:A:C8	2.38	0.58
1:A:203:G:N2	1:A:204:G:O6	2.35	0.58
22:a:72:U:OP2	45:x:54:LYS:NZ	2.28	0.58
1:A:715:A:H2'	1:A:716:A:C8	2.39	0.58
22:a:494:G:H4'	39:r:6:LYS:HB2	1.85	0.58
22:a:1432:G:H2'	22:a:1433:A:C8	2.38	0.58
1:A:147:G:H2'	1:A:148:G:C8	2.39	0.58
42:u:51:GLN:HG2	42:u:86:LEU:HD11	1.85	0.58
22:a:5:A:H2'	22:a:6:A:C8	2.39	0.58
23:b:36:C:O2'	23:b:37:C:OP1	2.19	0.58
1:A:337:G:H2'	1:A:338:A:H8	1.68	0.57
1:A:1026:G:H1	1:A:1035:A:H61	1.51	0.57
9:I:21:ILE:HG12	9:I:63:LEU:HG	1.86	0.57
12:L:55:VAL:HG21	12:L:80:ILE:HD11	1.84	0.57
22:a:1997:C:OP2	25:d:129:THR:OG1	2.22	0.57
33:l:42:THR:HG22	33:l:93:VAL:HG12	1.87	0.57
22:a:5:A:H2'	22:a:6:A:H8	1.69	0.57
22:a:581:C:H2'	22:a:582:A:C8	2.38	0.57
22:a:1433:A:H2'	22:a:1434:A:C8	2.39	0.57
1:A:1004:A:H2'	1:A:1005:A:O4'	2.04	0.57
10:J:52:LEU:HA	10:J:62:ARG:HB3	1.86	0.57
1:A:938:A:N3	1:A:1376:U:O2'	2.32	0.57
22:a:277:G:OP2	22:a:277:G:N2	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:527:C:N4	22:a:2777:G:O2'	2.31	0.57
42:u:72:VAL:HG12	42:u:93:ARG:HA	1.86	0.57
1:A:1343:G:N3	9:I:123:ARG:NH1	2.53	0.57
22:a:1597:A:H5''	22:a:1598:A:H5'	1.87	0.57
1:A:1218:C:H2'	1:A:1219:A:C8	2.39	0.57
5:E:72:ILE:HD13	5:E:141:ILE:HG23	1.86	0.57
27:f:62:GLY:O	27:f:95:ARG:NH2	2.38	0.57
22:a:1378:A:O2'	22:a:1379:U:OP2	2.23	0.56
1:A:458:U:H3	1:A:474:G:H1	1.53	0.56
22:a:948:C:H2'	22:a:949:G:H8	1.69	0.56
22:a:2419:U:H4'	48:0:22:THR:HG21	1.87	0.56
1:A:1218:C:H2'	1:A:1219:A:H8	1.71	0.56
1:A:1522:U:H2'	1:A:1523:G:H8	1.70	0.56
10:J:10:LEU:HD11	10:J:25:ILE:HD12	1.88	0.56
15:O:64:ARG:NH1	15:O:68:ASP:OD1	2.38	0.56
39:r:2:GLU:HG2	39:r:108:SER:HB3	1.86	0.56
1:A:501:C:H2'	1:A:502:A:C8	2.40	0.56
12:L:34:CYS:HA	12:L:55:VAL:HG22	1.87	0.56
22:a:693:A:O2'	22:a:1353:A:N3	2.37	0.56
22:a:2859:G:H2'	22:a:2860:A:C8	2.41	0.56
31:j:40:LYS:HE3	31:j:57:VAL:HG12	1.86	0.56
22:a:1808:A:H3'	22:a:1809:A:C8	2.40	0.56
1:A:981:U:OP1	14:N:9:ARG:NH1	2.38	0.56
11:K:28:ASN:O	11:K:57:LYS:NZ	2.36	0.56
22:a:748:G:OP2	59:a:6197:SPD:N10	2.35	0.56
22:a:576:U:H2'	22:a:577:G:C8	2.41	0.56
22:a:671:C:OP1	32:k:43:GLY:N	2.37	0.56
22:a:1385:A:O2'	22:a:1396:U:O2	2.23	0.56
22:a:181:A:H1'	22:a:435:C:H5'	1.88	0.56
22:a:1819:A:H5''	24:c:160:THR:HG21	1.88	0.56
1:A:999:C:H2'	1:A:1000:A:C8	2.40	0.56
22:a:2581:G:OP2	22:a:2581:G:N2	2.32	0.56
1:A:923:A:O2'	1:A:1399:C:OP2	2.25	0.55
22:a:1434:A:H2'	22:a:1435:G:H8	1.70	0.55
26:e:16:GLU:O	26:e:20:GLY:CA	2.54	0.55
19:S:28:LYS:NZ	19:S:46:GLY:O	2.37	0.55
22:a:1429:G:H2'	22:a:1430:G:H8	1.70	0.55
22:a:2575:C:H5'	25:d:149:ASN:HB2	1.89	0.55
20:T:42:GLY:HA2	20:T:86:LEU:HD11	1.88	0.55
23:b:5:U:OP1	23:b:61:G:O2'	2.22	0.55
1:A:202:G:O2'	1:A:468:A:N3	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:16:LEU:HG	21:U:20:LYS:HE2	1.88	0.55
22:a:1796:U:H2'	22:a:1797:G:H8	1.71	0.55
22:a:1353:A:H2'	22:a:1354:A:C8	2.42	0.55
34:m:12:ARG:O	34:m:17:ARG:NH1	2.39	0.55
1:A:1229:A:OP2	13:M:113:ARG:NH2	2.39	0.55
4:D:202:GLU:OE1	5:E:112:ARG:NH1	2.35	0.55
30:i:13:ARG:NH2	30:i:49:ASP:O	2.38	0.55
22:a:1447:C:O2'	22:a:1544:A:N3	2.33	0.55
22:a:2215:C:H2'	22:a:2216:G:H8	1.71	0.55
2:B:68:LEU:HD11	2:B:92:VAL:HG23	1.89	0.55
10:J:52:LEU:HD23	10:J:62:ARG:HB3	1.89	0.55
30:i:1:MET:SD	30:i:1:MET:N	2.80	0.55
1:A:1359:C:OP2	14:N:75:ARG:NH1	2.41	0.54
3:C:14:ILE:HG22	3:C:15:VAL:HG13	1.89	0.54
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.89	0.54
17:Q:27:ARG:HG3	17:Q:40:ARG:HB2	1.87	0.54
22:a:828:U:H2'	22:a:829:A:C8	2.42	0.54
1:A:1162:C:H2'	1:A:1163:A:H8	1.71	0.54
22:a:463:G:N2	22:a:466:A:OP2	2.30	0.54
1:A:514:C:H2'	1:A:515:G:H8	1.72	0.54
39:r:4:ILE:HG22	39:r:106:VAL:HG22	1.90	0.54
44:w:59:ILE:HG12	44:w:67:VAL:HG21	1.87	0.54
1:A:1003:G:H21	1:A:1005:A:H5'	1.73	0.54
22:a:171:U:H2'	22:a:172:A:H8	1.72	0.54
22:a:219:A:N3	22:a:234:U:O2'	2.33	0.54
22:a:2328:A:H2'	22:a:2329:U:C6	2.42	0.54
22:a:2845:U:H5''	36:o:52:ASN:O	2.08	0.54
1:A:4:U:H2'	1:A:5:U:H2'	1.90	0.54
1:A:1013:G:N2	1:A:1016:A:OP2	2.35	0.54
12:L:50:ARG:HE	12:L:89:D2T:H6	1.73	0.54
22:a:155:A:H2'	22:a:156:A:C8	2.43	0.54
22:a:652:U:H5''	22:a:653:U:H2'	1.89	0.54
22:a:1716:U:H2'	22:a:1717:A:H8	1.73	0.54
22:a:1796:U:H2'	22:a:1797:G:C8	2.43	0.54
22:a:2192:U:H2'	22:a:2193:G:H8	1.73	0.54
1:A:28:A:O2'	1:A:296:U:OP1	2.25	0.54
13:M:90:ARG:HB2	13:M:97:VAL:HG13	1.89	0.54
22:a:2071:A:H2'	22:a:2072:C:C6	2.42	0.54
1:A:254:G:O2'	17:Q:18:GLU:O	2.26	0.54
1:A:1250:A:H2'	1:A:1251:A:C8	2.43	0.54
22:a:1353:A:H2'	22:a:1354:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1664:A:H61	22:a:1996:C:H42	1.56	0.54
22:a:2086:U:H2'	22:a:2087:G:C8	2.43	0.54
22:a:675:A:N3	22:a:2443:C:O2'	2.41	0.53
10:J:87:LEU:HD22	10:J:100:ILE:HD13	1.91	0.53
22:a:554:U:H2'	22:a:555:G:O4'	2.08	0.53
22:a:580:U:H2'	22:a:581:C:C6	2.43	0.53
22:a:1434:A:H2'	22:a:1435:G:C8	2.43	0.53
22:a:1754:A:N1	22:a:2716:C:O2'	2.36	0.53
22:a:2377:A:O2'	35:n:117:PHE:O	2.22	0.53
37:p:97:ASP:OD2	38:q:13:ARG:NH2	2.39	0.53
22:a:373:U:H2'	22:a:374:A:H8	1.71	0.53
22:a:1231:U:H2'	22:a:1232:G:H8	1.73	0.53
1:A:1391:U:H2'	1:A:1392:G:C8	2.43	0.53
17:Q:46:VAL:HG21	17:Q:61:ILE:HG21	1.90	0.53
22:a:1007:C:OP1	30:i:37:ARG:NH1	2.39	0.53
22:a:1645:G:H5''	22:a:1646:C:H5'	1.91	0.53
1:A:171:A:H2'	1:A:172:A:C8	2.43	0.53
22:a:1248:G:OP1	26:e:44:ARG:NH1	2.40	0.53
22:a:2836:U:H2'	22:a:2837:A:C8	2.44	0.53
16:P:8:ARG:O	16:P:29:ASN:ND2	2.41	0.53
22:a:672:C:OP2	32:k:42:SER:OG	2.26	0.53
22:a:910:A:H2'	22:a:911:A:C8	2.44	0.53
22:a:1114:C:H2'	22:a:1115:G:C8	2.43	0.53
32:k:77:ILE:HD13	32:k:108:ALA:HB1	1.89	0.53
1:A:150:U:H2'	1:A:151:A:H8	1.73	0.53
1:A:552:U:H2'	1:A:553:A:H8	1.73	0.53
18:R:36:SER:HA	18:R:72:ASP:HB3	1.91	0.53
3:C:138:VAL:HA	3:C:149:ILE:HD13	1.91	0.53
20:T:35:VAL:HG11	20:T:79:LEU:HD13	1.91	0.53
22:a:880:G:H3'	22:a:881:G:H5''	1.91	0.53
46:y:9:GLN:HB2	46:y:29:LEU:HD13	1.91	0.53
50:2:16:LYS:HE3	50:2:20:GLY:HA2	1.90	0.53
22:a:172:A:H2'	22:a:173:A:H8	1.74	0.53
22:a:177:G:OP2	22:a:177:G:N2	2.24	0.53
22:a:639:U:H2'	22:a:640:C:C6	2.44	0.53
22:a:1744:A:H3'	22:a:1745:A:H8	1.73	0.53
22:a:2366:A:H4'	43:v:62:LYS:HE3	1.91	0.53
1:A:34:C:H2'	1:A:35:G:H8	1.74	0.53
1:A:811:C:O2'	1:A:901:A:N1	2.41	0.53
5:E:81:LEU:HB2	5:E:98:PRO:HG3	1.91	0.53
22:a:191:A:H2'	22:a:192:C:H6	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2014:A:H2'	22:a:2015:A:C8	2.43	0.53
42:u:1:MET:HE1	42:u:53:LYS:HD3	1.91	0.53
55:Y:23:A:H2'	55:Y:24:A:C8	2.44	0.53
1:A:999:C:H2'	1:A:1000:A:H8	1.74	0.52
1:A:1228:C:H1'	13:M:116:ILE:HD11	1.91	0.52
11:K:64:GLN:HG3	11:K:99:ALA:HB2	1.91	0.52
17:Q:11:ARG:HE	17:Q:56:GLY:HA2	1.74	0.52
22:a:360:U:H3'	22:a:361:G:C8	2.44	0.52
22:a:1667:G:O2'	22:a:1991:U:O4	2.24	0.52
1:A:662:U:H2'	1:A:663:A:C8	2.44	0.52
1:A:712:A:H2'	1:A:713:G:C8	2.43	0.52
1:A:1167:A:O2'	1:A:1169:A:N7	2.41	0.52
22:a:239:C:O2'	22:a:622:G:O2'	2.22	0.52
22:a:365:U:H2'	22:a:366:C:C6	2.45	0.52
22:a:1746:A:H2'	22:a:1747:U:C6	2.44	0.52
22:a:2657:A:O2'	28:g:160:LYS:NZ	2.43	0.52
1:A:390:U:H2'	1:A:391:G:H8	1.73	0.52
22:a:2329:U:H2'	22:a:2330:G:C8	2.44	0.52
22:a:2723:C:OP1	25:d:114:LYS:NZ	2.41	0.52
1:A:1071:C:H2'	1:A:1072:G:C8	2.43	0.52
4:D:102:VAL:HG21	4:D:123:ILE:HD13	1.89	0.52
22:a:753:A:H2'	22:a:754:U:H6	1.74	0.52
22:a:1028:A:H2'	22:a:1029:A:C8	2.44	0.52
41:t:26:LYS:HE3	41:t:37:GLU:HB2	1.91	0.52
11:K:111:THR:HG23	21:U:3:VAL:HG22	1.91	0.52
22:a:2731:G:H2'	22:a:2732:G:C8	2.44	0.52
32:k:57:LEU:HD22	50:2:54:ASP:HB3	1.90	0.52
1:A:1130:A:H61	1:A:1144:G:H1'	1.73	0.52
21:U:4:ILE:HD13	21:U:19:PHE:HD1	1.74	0.52
22:a:1223:G:OP1	38:q:68:ARG:NH1	2.42	0.52
1:A:1524:C:H2'	1:A:1525:G:C8	2.45	0.52
7:G:126:ASP:HA	7:G:129:GLU:HG2	1.92	0.52
22:a:521:U:H2'	22:a:522:A:C8	2.44	0.52
22:a:1028:A:N3	22:a:2486:C:O2'	2.38	0.52
22:a:1292:G:H2'	22:a:1293:C:H6	1.75	0.52
22:a:2216:G:H2'	22:a:2217:G:H8	1.75	0.52
1:A:337:G:H2'	1:A:338:A:C8	2.45	0.52
1:A:390:U:H2'	1:A:391:G:C8	2.45	0.52
1:A:1373:G:H5''	7:G:36:LYS:HD2	1.92	0.52
22:a:1847:A:H4'	22:a:1848:A:OP1	2.10	0.52
25:d:152:PRO:HB2	25:d:154:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:e:129:PRO:HB3	26:e:156:ASN:HA	1.91	0.52
1:A:1027:C:N3	1:A:1028:C:N4	2.57	0.52
1:A:1144:G:H2'	1:A:1145:A:C8	2.45	0.52
1:A:1287:A:H2'	1:A:1288:A:C8	2.45	0.52
1:A:1524:C:H2'	1:A:1525:G:H8	1.75	0.52
3:C:24:ALA:HB1	3:C:28:GLU:HG2	1.92	0.52
22:a:993:G:OP2	37:p:51:ARG:NH2	2.41	0.52
22:a:1438:U:H2'	22:a:1439:A:H8	1.75	0.52
22:a:2291:U:H2'	22:a:2292:U:C6	2.45	0.52
22:a:2591:C:H2'	22:a:2592:G:C8	2.45	0.52
22:a:354:A:H2'	22:a:355:U:O4'	2.09	0.51
22:a:355:U:H2'	22:a:356:G:H8	1.75	0.51
22:a:665:U:H2'	22:a:666:A:H8	1.75	0.51
1:A:294:U:OP1	1:A:610:U:O2'	2.26	0.51
1:A:532:A:N6	1:A:1206:G:O2'	2.43	0.51
1:A:1001:C:H2'	1:A:1002:G:H8	1.75	0.51
22:a:1013:C:H2'	22:a:1014:A:H8	1.75	0.51
1:A:41:G:H2'	1:A:42:G:H8	1.74	0.51
1:A:217:C:H2'	1:A:218:U:C6	2.45	0.51
3:C:70:THR:HG21	3:C:76:VAL:HG21	1.92	0.51
22:a:166:U:H2'	22:a:167:A:H8	1.75	0.51
48:0:35:GLU:HG2	48:0:50:LYS:HG2	1.93	0.51
1:A:131:A:H2'	1:A:132:C:C6	2.45	0.51
22:a:645:C:H2'	22:a:647:G:C8	2.45	0.51
22:a:1278:C:H2'	22:a:1279:G:H8	1.75	0.51
22:a:2698:U:H2'	22:a:2699:C:C6	2.46	0.51
27:f:44:ILE:HG21	27:f:79:ILE:HG22	1.91	0.51
1:A:524:G:H2'	1:A:525:C:C6	2.45	0.51
1:A:976:G:OP2	1:A:1358:U:O2'	2.28	0.51
3:C:19:ASN:O	3:C:40:ARG:NH2	2.43	0.51
22:a:30:G:O2'	22:a:1214:A:N3	2.42	0.51
22:a:582:A:H2'	22:a:583:G:H8	1.76	0.51
1:A:50:A:O2'	1:A:360:G:N2	2.43	0.51
4:D:104:ARG:HB3	4:D:168:PRO:HG2	1.93	0.51
22:a:2847:U:H2'	22:a:2848:G:O4'	2.10	0.51
42:u:30:ILE:HG12	42:u:91:PHE:HB2	1.92	0.51
55:Y:63:C:H2'	55:Y:64:G:H8	1.76	0.51
1:A:652:U:O4	1:A:752:G:O2'	2.23	0.51
1:A:1308:U:H2'	1:A:1309:G:H8	1.76	0.51
1:A:1314:C:H2'	1:A:1315:U:C6	2.46	0.51
22:a:473:G:OP2	59:a:6196:SPD:N10	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1361:G:H2'	22:a:1362:C:C6	2.45	0.51
31:j:43:ILE:HD12	31:j:56:ASP:HB2	1.92	0.51
4:D:44:ARG:HG3	4:D:46:PRO:HD3	1.93	0.51
7:G:66:LEU:O	7:G:70:ARG:HB2	2.11	0.51
22:a:755:U:H2'	22:a:756:A:C8	2.46	0.51
22:a:1443:U:H2'	22:a:1444:G:H8	1.76	0.51
27:f:103:LEU:HD12	27:f:107:ALA:HB3	1.93	0.51
28:g:24:ILE:HD13	28:g:72:LEU:HD21	1.92	0.51
28:g:127:THR:OG1	28:g:130:GLU:OE1	2.29	0.51
22:a:155:A:H2'	22:a:156:A:H8	1.74	0.51
22:a:1141:U:H4'	22:a:1142:A:O4'	2.11	0.51
22:a:1529:G:H1	22:a:1542:U:H3	1.58	0.51
22:a:2591:C:H2'	22:a:2592:G:H8	1.76	0.51
22:a:302:C:H2'	22:a:303:G:H8	1.75	0.50
22:a:703:U:H2'	22:a:704:G:O4'	2.11	0.50
22:a:2215:C:H2'	22:a:2216:G:C8	2.45	0.50
1:A:1414:U:H2'	1:A:1415:G:H8	1.76	0.50
6:F:43:GLY:HA2	6:F:58:HIS:CE1	2.47	0.50
22:a:2469:A:H4'	33:l:55:ARG:HD2	1.93	0.50
1:A:674:G:H2'	1:A:675:A:C8	2.44	0.50
1:A:816:A:OP1	1:A:1526:G:O2'	2.28	0.50
1:A:1513:A:H2'	1:A:1514:G:C8	2.46	0.50
10:J:76:ILE:HG21	10:J:83:THR:HG21	1.93	0.50
13:M:7:ILE:HD11	13:M:22:ILE:HG12	1.93	0.50
22:a:593:U:H2'	22:a:594:U:C6	2.47	0.50
28:g:89:LEU:HD22	28:g:162:VAL:HG22	1.91	0.50
12:L:42:PRO:HB3	12:L:89:D2T:SB	2.51	0.50
22:a:358:U:H2'	22:a:359:G:H8	1.75	0.50
28:g:52:PHE:HE2	28:g:72:LEU:HD22	1.76	0.50
9:I:130:ARG:NH1	55:Y:33:U:OP2	2.36	0.50
22:a:729:G:H5'	22:a:730:A:H5''	1.93	0.50
22:a:1223:G:N2	22:a:1226:A:OP2	2.33	0.50
22:a:1315:C:O2'	22:a:1392:A:N3	2.39	0.50
22:a:1361:G:H2'	22:a:1362:C:H6	1.77	0.50
22:a:1548:A:H2'	22:a:1549:A:C8	2.47	0.50
22:a:2547:A:H2'	22:a:2548:U:C6	2.47	0.50
1:A:56:U:H2'	1:A:57:G:H8	1.76	0.50
1:A:358:U:H2'	1:A:359:G:H8	1.76	0.50
1:A:746:A:H2'	1:A:747:A:C8	2.46	0.50
1:A:1142:G:C2	1:A:1143:G:H1'	2.46	0.50
22:a:2836:U:H2'	22:a:2837:A:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:l:75:GLU:HB2	33:l:90:GLU:HG3	1.93	0.50
1:A:1356:G:H2'	1:A:1357:A:C8	2.46	0.50
4:D:61:VAL:HG21	4:D:200:ILE:HD11	1.93	0.50
22:a:827:U:O2'	22:a:2068:U:N3	2.45	0.50
22:a:888:C:H2'	22:a:889:C:O4'	2.12	0.50
1:A:216:U:H2'	1:A:217:C:C6	2.47	0.50
4:D:105:MET:HE1	4:D:143:VAL:HB	1.94	0.50
12:L:110:ARG:HB3	12:L:119:VAL:HG21	1.94	0.50
22:a:1720:U:H2'	22:a:1721:G:O4'	2.11	0.50
22:a:1727:C:H2'	22:a:1728:C:O4'	2.11	0.50
22:a:1839:G:C2	22:a:1840:G:C8	3.00	0.50
1:A:41:G:H2'	1:A:42:G:C8	2.47	0.50
1:A:539:A:H2'	1:A:540:G:C8	2.47	0.50
1:A:1003:G:N2	1:A:1005:A:H5'	2.25	0.50
1:A:1226:C:OP2	13:M:102:THR:OG1	2.19	0.50
2:B:214:LEU:HA	2:B:217:VAL:HG22	1.92	0.50
22:a:2515:C:H2'	22:a:2516:A:H8	1.76	0.50
1:A:501:C:OP1	12:L:114:ARG:NH2	2.36	0.49
22:a:1153:C:OP1	37:p:92:ARG:NH2	2.41	0.49
22:a:1563:U:H2'	22:a:1564:C:C6	2.46	0.49
22:a:1564:C:H2'	22:a:1565:C:C6	2.47	0.49
22:a:1864:U:OP1	22:a:2410:G:O2'	2.26	0.49
22:a:2788:C:H2'	22:a:2789:C:C6	2.47	0.49
26:e:149:ILE:HG22	26:e:192:ALA:HB1	1.92	0.49
30:i:125:TYR:OH	30:i:132:HIS:NE2	2.36	0.49
1:A:1439:G:OP2	20:T:33:LYS:NZ	2.43	0.49
22:a:1746:A:H2'	22:a:1747:U:H6	1.76	0.49
22:a:1853:A:H2'	22:a:1854:A:C8	2.47	0.49
28:g:26:ILE:HD11	28:g:75:MET:HB3	1.93	0.49
22:a:358:U:H2'	22:a:359:G:C8	2.47	0.49
22:a:657:U:H2'	22:a:658:U:C6	2.47	0.49
22:a:927:A:H2'	22:a:928:A:C8	2.48	0.49
22:a:1682:G:H2'	22:a:1683:U:C6	2.46	0.49
39:r:20:VAL:HG11	39:r:44:ALA:HA	1.94	0.49
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.94	0.49
9:I:19:VAL:HG13	9:I:65:ILE:HG12	1.94	0.49
18:R:32:TYR:O	18:R:40:VAL:HG22	2.12	0.49
1:A:235:C:H2'	1:A:236:A:H8	1.78	0.49
1:A:579:A:H2'	1:A:580:C:C6	2.48	0.49
1:A:1011:C:H2'	1:A:1012:A:C8	2.48	0.49
1:A:1363:A:O2'	1:A:1365:G:N7	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:250:G:O2'	22:a:251:A:OP1	2.27	0.49
31:j:7:MET:HE1	31:j:44:LYS:HG3	1.94	0.49
35:n:51:ALA:HB3	35:n:78:VAL:HB	1.94	0.49
22:a:1856:U:H2'	22:a:1857:G:O4'	2.13	0.49
22:a:2008:C:H2'	22:a:2009:A:H8	1.78	0.49
28:g:159:GLY:O	28:g:163:ARG:NH2	2.37	0.49
22:a:1000:A:H2'	22:a:1001:A:C8	2.48	0.49
22:a:2618:G:H21	25:d:155:VAL:HG21	1.78	0.49
27:f:36:LEU:HD22	27:f:154:ILE:HG12	1.94	0.49
1:A:600:A:H2'	1:A:601:G:H8	1.78	0.49
1:A:1077:G:N2	1:A:1080:A:OP2	2.37	0.49
2:B:95:ARG:HH11	2:B:97:LEU:HD23	1.77	0.49
13:M:34:LEU:HD13	13:M:41:GLU:HA	1.95	0.49
22:a:1149:G:H2'	22:a:1150:C:C6	2.48	0.49
22:a:1901:A:OP2	24:c:253:LYS:NZ	2.39	0.49
22:a:2705:A:O2'	22:a:2852:G:OP1	2.26	0.49
22:a:1794:A:H2'	22:a:1795:C:C6	2.47	0.49
22:a:2081:U:H2'	22:a:2082:A:H8	1.76	0.49
32:k:132:ARG:HG3	32:k:142:ILE:HD12	1.94	0.49
42:u:7:GLU:HB2	42:u:41:GLU:HG3	1.95	0.49
1:A:1140:C:H2'	1:A:1141:C:C6	2.47	0.49
13:M:83:LEU:HD21	19:S:65:GLU:HB2	1.94	0.49
15:O:36:ILE:O	15:O:40:GLN:HG2	2.12	0.49
22:a:629:G:H1'	22:a:639:U:H1'	1.95	0.49
35:n:39:VAL:HB	35:n:49:VAL:HB	1.95	0.49
37:p:40:ILE:HG22	37:p:44:GLN:HE21	1.77	0.49
22:a:521:U:H2'	22:a:522:A:H8	1.78	0.48
22:a:582:A:H2'	22:a:583:G:C8	2.48	0.48
22:a:947:A:H2'	22:a:948:C:C6	2.48	0.48
22:a:1737:G:H2'	22:a:1738:G:H1'	1.94	0.48
22:a:2298:A:OP1	27:f:71:ARG:NH1	2.45	0.48
55:Y:65:U:H2'	55:Y:66:C:C6	2.48	0.48
1:A:648:A:H2'	1:A:649:A:C8	2.48	0.48
22:a:296:U:H2'	22:a:297:G:C8	2.48	0.48
38:q:34:GLU:HG3	38:q:58:VAL:HG13	1.94	0.48
1:A:460:A:H2'	1:A:461:A:H8	1.78	0.48
22:a:2573:C:OP1	22:a:2574:G:OP1	2.30	0.48
33:l:25:ASP:O	33:l:66:ARG:NH1	2.45	0.48
41:t:4:LYS:O	41:t:94:ARG:NH1	2.46	0.48
52:4:11:GLU:HA	52:4:25:ARG:HA	1.94	0.48
1:A:1513:A:H2'	1:A:1514:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:H	2:B:100:MET:HE3	1.78	0.48
5:E:148:ASN:HD22	8:H:96:MET:HE1	1.78	0.48
22:a:1570:A:H2'	22:a:1571:A:C8	2.48	0.48
22:a:1672:A:C2	22:a:2582:G:H5'	2.48	0.48
22:a:2223:G:O2'	24:c:265:LYS:NZ	2.31	0.48
22:a:2405:G:O2'	22:a:2411:A:N6	2.46	0.48
23:b:60:C:H2'	23:b:61:G:H8	1.78	0.48
44:w:12:PRO:HB3	44:w:30:LEU:HD23	1.95	0.48
1:A:1000:A:H2'	1:A:1001:C:C6	2.48	0.48
22:a:1306:C:H2'	22:a:1307:A:H8	1.78	0.48
22:a:1469:A:H2'	22:a:1470:A:C8	2.49	0.48
36:o:51:ARG:HG2	36:o:53:ARG:HG2	1.96	0.48
1:A:1028:C:H2'	1:A:1029:U:O4'	2.12	0.48
22:a:2532:G:N2	22:a:2663:G:O2'	2.46	0.48
22:a:2589:A:H2'	22:a:2590:A:H8	1.78	0.48
22:a:2687:U:H2'	22:a:2688:G:O4'	2.14	0.48
33:l:11:LYS:HD3	33:l:86:LYS:HD3	1.95	0.48
1:A:127:G:O2'	17:Q:6:ARG:NH1	2.46	0.48
1:A:1118:U:H1'	1:A:1179:A:C5	2.48	0.48
1:A:1314:C:H2'	1:A:1315:U:H6	1.77	0.48
10:J:80:THR:HG23	10:J:83:THR:H	1.79	0.48
22:a:1709:U:H2'	22:a:1710:G:C8	2.49	0.48
22:a:2812:G:H2'	22:a:2813:A:H8	1.79	0.48
30:i:114:LEU:HG	30:i:118:MET:HE3	1.95	0.48
1:A:471:U:H2'	1:A:472:U:H6	1.79	0.48
1:A:1095:U:H2'	1:A:1096:C:C6	2.49	0.48
1:A:1255:G:O2'	1:A:1258:G:N3	2.39	0.48
2:B:67:ILE:O	2:B:89:GLN:HB3	2.12	0.48
42:u:26:PHE:HZ	42:u:47:VAL:HG11	1.78	0.48
1:A:464:U:N3	1:A:467:U:OP2	2.45	0.48
1:A:1488:G:H2'	1:A:1489:G:H8	1.79	0.48
22:a:2258:C:O2'	22:a:2427:C:OP2	2.32	0.48
22:a:2637:U:H2'	22:a:2638:G:O4'	2.13	0.48
55:Y:8:U:O2'	55:Y:21:A:N1	2.36	0.48
1:A:1063:C:OP2	1:A:1064:G:O2'	2.29	0.48
6:F:90:MET:SD	18:R:61:ARG:NH1	2.87	0.48
22:a:767:U:H2'	22:a:768:G:H8	1.79	0.48
22:a:1198:U:H2'	22:a:1199:U:C6	2.49	0.48
22:a:1847:A:O2'	22:a:1848:A:O5'	2.29	0.48
22:a:2020:A:H5'	47:z:9:THR:HG21	1.94	0.48
1:A:346:G:OP1	36:o:39:ARG:NH1	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:A:H2'	1:A:1013:G:C8	2.49	0.47
1:A:1034:G:H2'	1:A:1035:A:C8	2.46	0.47
1:A:1148:U:H2'	1:A:1149:C:O4'	2.13	0.47
4:D:100:ASN:HD22	4:D:111:ARG:HE	1.62	0.47
22:a:411:G:OP2	22:a:2406:A:O2'	2.24	0.47
22:a:2025:C:H2'	22:a:2026:U:C6	2.48	0.47
4:D:78:GLU:OE2	4:D:81:ARG:NH2	2.43	0.47
22:a:1292:G:H2'	22:a:1293:C:C6	2.50	0.47
22:a:2037:A:H2'	22:a:2038:G:C8	2.49	0.47
22:a:2071:A:H1'	59:a:6199:SPD:H91	1.95	0.47
22:a:2898:U:H2'	22:a:2899:A:H8	1.79	0.47
36:o:33:VAL:HG22	36:o:38:LYS:HG3	1.96	0.47
55:Y:63:C:H2'	55:Y:64:G:C8	2.49	0.47
1:A:744:C:H2'	1:A:745:G:C8	2.43	0.47
14:N:27:LEU:HD21	14:N:47:LYS:HD3	1.95	0.47
20:T:20:HIS:O	20:T:24:ARG:HG2	2.14	0.47
22:a:58:G:O2'	22:a:73:A:N1	2.46	0.47
22:a:151:C:H2'	22:a:152:A:H8	1.78	0.47
22:a:264:C:O2'	22:a:265:A:O5'	2.27	0.47
22:a:2837:A:H2'	22:a:2838:G:H8	1.79	0.47
23:b:79:G:O6	42:u:14:LYS:NZ	2.39	0.47
1:A:1217:C:OP2	14:N:9:ARG:NH2	2.43	0.47
10:J:54:SER:OG	10:J:58:ASN:HB2	2.14	0.47
22:a:69:C:O2	22:a:73:A:O2'	2.27	0.47
22:a:2070:A:H2'	22:a:2071:A:C8	2.49	0.47
23:b:1:U:H2'	23:b:2:G:H8	1.79	0.47
24:c:260:ASN:ND2	24:c:263:THR:OG1	2.47	0.47
29:h:56:ALA:O	29:h:60:GLU:HG2	2.15	0.47
1:A:994:A:C4	1:A:1216:A:H4'	2.49	0.47
1:A:1238:A:H2	1:A:1241:G:N3	2.13	0.47
22:a:419:U:H2'	22:a:420:C:C6	2.49	0.47
22:a:807:U:OP2	32:k:41:ARG:NH2	2.46	0.47
22:a:2780:G:OP2	30:i:120:ARG:HD3	2.15	0.47
24:c:3:VAL:HG12	24:c:19:VAL:HG22	1.96	0.47
32:k:79:LEU:HB3	32:k:116:VAL:HG23	1.97	0.47
33:l:21:ALA:HB2	33:l:97:GLN:HB2	1.97	0.47
37:p:86:ALA:HB2	37:p:116:ALA:HB2	1.97	0.47
4:D:15:GLU:OE2	4:D:63:ARG:NH1	2.47	0.47
14:N:53:ARG:HB3	14:N:59:ARG:HH11	1.79	0.47
22:a:32:C:H2'	22:a:33:C:C6	2.49	0.47
22:a:635:C:O2'	22:a:639:U:OP1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:742:A:H2'	22:a:743:A:C8	2.50	0.47
22:a:1442:U:H2'	22:a:1443:U:C6	2.50	0.47
22:a:2502:G:H5''	22:a:2503:2MA:H5''	1.95	0.47
22:a:2567:G:H2'	22:a:2568:U:C6	2.50	0.47
22:a:2751:G:OP2	28:g:3:ARG:NH1	2.47	0.47
44:w:43:GLU:OE1	44:w:45:ARG:NE	2.42	0.47
1:A:859:G:H2'	1:A:860:A:C8	2.50	0.47
1:A:1412:C:H2'	1:A:1413:A:C8	2.50	0.47
2:B:115:LYS:O	2:B:118:GLU:HG2	2.14	0.47
11:K:31:ILE:HG12	11:K:46:THR:HG22	1.96	0.47
22:a:447:A:O2'	59:a:6196:SPD:N10	2.47	0.47
22:a:589:U:H2'	22:a:590:A:C8	2.49	0.47
22:a:945:A:N3	59:a:6193:SPD:H71	2.30	0.47
22:a:1709:U:H2'	22:a:1710:G:H8	1.79	0.47
22:a:2199:A:N1	22:a:2226:C:N4	2.61	0.47
22:a:2850:A:N7	22:a:2868:A:O2'	2.38	0.47
23:b:34:A:H5'	23:b:35:C:OP1	2.15	0.47
38:q:61:ALA:HB2	38:q:98:ILE:HD13	1.97	0.47
39:r:3:THR:OG1	39:r:62:ASP:OD2	2.27	0.47
40:s:11:LEU:O	45:x:29:ARG:NH2	2.48	0.47
1:A:746:A:H2'	1:A:747:A:H8	1.79	0.47
9:I:54:LEU:HD23	9:I:98:LEU:HD23	1.96	0.47
17:Q:19:LYS:H	17:Q:51:ASN:ND2	2.13	0.47
22:a:249:C:H4'	22:a:250:G:O5'	2.15	0.47
1:A:1149:C:H2'	1:A:1150:A:C8	2.43	0.47
1:A:1507:A:H2'	1:A:1508:A:C8	2.49	0.47
5:E:148:ASN:ND2	8:H:73:GLU:OE2	2.48	0.47
22:a:1814:G:OP2	22:a:1815:A:O2'	2.28	0.47
22:a:2372:U:H2'	22:a:2373:G:H8	1.80	0.47
22:a:2430:A:N3	22:a:2430:A:H2'	2.29	0.47
31:j:102:PRO:HD3	36:o:66:ASN:HB2	1.97	0.47
1:A:908:A:H2'	1:A:909:A:H8	1.80	0.47
1:A:1183:U:O2'	1:A:1185:G:OP2	2.32	0.47
1:A:1219:A:H2'	1:A:1220:G:C8	2.49	0.47
2:B:161:LEU:HD22	2:B:176:ALA:HB2	1.96	0.47
22:a:1870:C:H3'	22:a:1871:A:H8	1.79	0.47
22:a:717:C:H3'	22:a:718:A:H8	1.80	0.46
22:a:2350:C:H2'	22:a:2351:G:O4'	2.15	0.46
27:f:16:LEU:HD13	27:f:29:PRO:HD2	1.96	0.46
1:A:470:C:H2'	1:A:471:U:H6	1.80	0.46
1:A:676:A:H5''	11:K:115:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:G:H2'	1:A:746:A:C8	2.50	0.46
6:F:6:ILE:HG12	6:F:89:VAL:HG22	1.97	0.46
7:G:59:LEU:O	7:G:63:GLU:HG2	2.15	0.46
22:a:598:U:H2'	22:a:599:A:H8	1.80	0.46
22:a:753:A:H2'	22:a:754:U:C6	2.51	0.46
22:a:1450:G:N2	22:a:1452:G:O6	2.24	0.46
42:u:48:MET:SD	42:u:51:GLN:NE2	2.86	0.46
1:A:17:U:H2'	1:A:18:C:C6	2.50	0.46
1:A:501:C:H1'	1:A:549:C:H1'	1.97	0.46
1:A:665:A:H1'	1:A:733:G:H5'	1.97	0.46
3:C:64:ILE:HG22	3:C:97:VAL:HG23	1.97	0.46
4:D:170:TRP:O	4:D:183:LYS:HG2	2.15	0.46
22:a:250:G:HO2'	22:a:251:A:P	2.38	0.46
22:a:639:U:H2'	22:a:640:C:H6	1.80	0.46
22:a:1587:G:H2'	22:a:1588:G:H8	1.80	0.46
36:o:75:GLN:HB2	36:o:78:SER:HB2	1.96	0.46
1:A:1347:G:O6	9:I:12:ARG:NH2	2.47	0.46
22:a:284:U:O4	22:a:356:G:O6	2.34	0.46
22:a:514:A:N3	22:a:581:C:O2'	2.46	0.46
22:a:1406:U:H2'	22:a:1407:G:C8	2.51	0.46
22:a:2243:U:H2'	22:a:2244:U:C6	2.50	0.46
1:A:1034:G:O2'	1:A:1035:A:H5'	2.16	0.46
22:a:1469:A:H2'	22:a:1470:A:H8	1.81	0.46
22:a:1802:A:H2'	22:a:1803:A:H8	1.79	0.46
22:a:2192:U:H2'	22:a:2193:G:C8	2.50	0.46
1:A:513:C:H2'	1:A:514:C:C6	2.51	0.46
1:A:1134:G:H2'	1:A:1135:U:O4'	2.16	0.46
4:D:177:LYS:HG3	4:D:179:GLU:HG2	1.96	0.46
5:E:13:GLU:HG2	5:E:39:VAL:HG12	1.97	0.46
22:a:1847:A:O2'	22:a:1848:A:H8	1.99	0.46
22:a:1847:A:HO2'	22:a:1848:A:C5'	2.29	0.46
22:a:2522:U:O2'	22:a:2647:U:OP1	2.28	0.46
25:d:136:ASN:ND2	25:d:139:SER:O	2.44	0.46
1:A:27:G:H2'	1:A:28:A:H8	1.79	0.46
1:A:176:C:H2'	1:A:177:G:N3	2.31	0.46
1:A:246:A:C2	1:A:282:A:C5	3.04	0.46
1:A:579:A:H5'	1:A:728:A:H1'	1.97	0.46
1:A:634:C:H2'	1:A:635:A:H8	1.80	0.46
1:A:1060:U:H2'	1:A:1061:G:H8	1.81	0.46
3:C:73:PRO:HG3	3:C:105:GLU:HG2	1.98	0.46
11:K:35:THR:HG22	11:K:41:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:36:G:N3	22:a:450:G:O2'	2.49	0.46
22:a:569:U:O2'	22:a:983:A:N1	2.48	0.46
22:a:1028:A:N6	22:a:1125:G:H2'	2.31	0.46
22:a:1046:A:H3'	22:a:1047:G:H5'	1.97	0.46
22:a:1636:U:H2'	22:a:1637:A:C8	2.51	0.46
22:a:2074:U:H2'	22:a:2075:U:C6	2.51	0.46
22:a:2229:U:H2'	22:a:2230:G:H8	1.80	0.46
22:a:2597:G:H2'	22:a:2598:A:C8	2.50	0.46
22:a:2799:A:O2'	22:a:2800:A:H5''	2.15	0.46
30:i:62:VAL:HG11	30:i:101:ILE:HD11	1.97	0.46
31:j:80:ASP:OD2	36:o:62:ARG:NH2	2.41	0.46
42:u:68:LYS:HE2	42:u:70:ILE:HG12	1.98	0.46
1:A:109:A:H5'	1:A:110:C:H5	1.80	0.46
1:A:335:C:H2'	1:A:336:A:C8	2.47	0.46
1:A:675:A:H1'	11:K:118:HIS:CG	2.51	0.46
22:a:720:U:H2'	22:a:721:A:C8	2.51	0.46
22:a:749:A:OP2	59:a:6197:SPD:N10	2.49	0.46
22:a:755:U:H2'	22:a:756:A:H8	1.80	0.46
22:a:1752:C:H2'	22:a:1753:G:C8	2.51	0.46
22:a:1969:A:H2'	22:a:1972:G:H21	1.81	0.46
22:a:2286:G:H4'	22:a:2287:A:O4'	2.16	0.46
27:f:29:PRO:HB3	27:f:160:ALA:HB2	1.98	0.46
43:v:59:LEU:HD12	43:v:80:ILE:HD12	1.98	0.46
7:G:26:PHE:HE2	7:G:120:LEU:HD21	1.81	0.46
22:a:94:A:H2'	22:a:95:A:C8	2.51	0.46
22:a:1429:G:H2'	22:a:1430:G:C8	2.50	0.46
22:a:1726:C:H2'	22:a:1727:C:C6	2.51	0.46
22:a:1794:A:H2'	22:a:1795:C:H6	1.80	0.46
22:a:1927:A:H2'	22:a:1928:A:C8	2.51	0.46
22:a:2250:G:O2'	22:a:2496:C:OP1	2.34	0.46
22:a:2557:G:H2'	22:a:2558:C:C6	2.50	0.46
33:l:6:ARG:NH2	55:Y:52:G:O3'	2.49	0.46
1:A:648:A:H2'	1:A:649:A:H8	1.80	0.46
1:A:1238:A:OP1	1:A:1335:U:O2'	2.22	0.46
22:a:445:C:H2'	22:a:446:G:O4'	2.16	0.46
22:a:764:A:H5'	24:c:209:GLY:HA2	1.98	0.46
22:a:1506:U:H2'	22:a:1507:C:C6	2.50	0.46
44:w:3:ARG:O	44:w:12:PRO:HD3	2.16	0.46
1:A:56:U:H2'	1:A:57:G:C8	2.51	0.45
1:A:1287:A:H2	1:A:1353:G:H1'	1.80	0.45
4:D:140:ASN:N	4:D:182:PHE:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1433:A:H2'	22:a:1434:A:H8	1.80	0.45
1:A:228:A:O2'	16:P:63:GLN:NE2	2.50	0.45
1:A:677:U:O2	1:A:777:A:O2'	2.32	0.45
7:G:115:SER:O	7:G:119:ARG:HG3	2.16	0.45
22:a:166:U:H2'	22:a:167:A:C8	2.50	0.45
22:a:172:A:H2'	22:a:173:A:C8	2.50	0.45
22:a:184:C:H2'	22:a:185:G:H8	1.80	0.45
22:a:302:C:H2'	22:a:303:G:C8	2.51	0.45
22:a:948:C:H2'	22:a:949:G:C8	2.51	0.45
22:a:1441:G:H2'	22:a:1442:U:C6	2.50	0.45
22:a:1604:C:O2'	22:a:1610:A:N1	2.43	0.45
22:a:1734:G:H2'	22:a:1735:A:H8	1.81	0.45
22:a:2282:G:H4'	22:a:2389:G:O2'	2.17	0.45
28:g:52:PHE:CE2	28:g:72:LEU:HD22	2.51	0.45
50:2:26:HIS:NE2	50:2:48:ALA:HB2	2.31	0.45
1:A:235:C:H2'	1:A:236:A:C8	2.51	0.45
1:A:1000:A:H2'	1:A:1001:C:H6	1.82	0.45
4:D:150:LYS:HA	4:D:178:MET:HE1	1.97	0.45
22:a:222:A:N6	22:a:232:G:H1'	2.31	0.45
22:a:2287:A:O5'	48:0:30:LYS:NZ	2.49	0.45
22:a:2514:U:H2'	22:a:2515:C:C6	2.51	0.45
26:e:149:ILE:HB	26:e:188:MET:HG2	1.99	0.45
51:3:16:ILE:HG12	51:3:25:VAL:HG22	1.99	0.45
6:F:12:PRO:O	6:F:44:ARG:NH2	2.49	0.45
22:a:244:A:OP2	50:2:8:ARG:NH2	2.49	0.45
22:a:673:C:OP1	26:e:49:ARG:NH1	2.49	0.45
22:a:2039:U:H2'	22:a:2040:G:C8	2.52	0.45
22:a:2812:G:H2'	22:a:2813:A:C8	2.50	0.45
28:g:19:ILE:HG12	28:g:24:ILE:HD12	1.98	0.45
48:0:11:LEU:HD21	48:0:34:LEU:HD23	1.99	0.45
52:4:28:VAL:HG11	52:4:32:LEU:HD21	1.96	0.45
1:A:191:G:H2'	1:A:192:A:H8	1.82	0.45
1:A:945:G:C2	1:A:946:A:C8	3.04	0.45
6:F:32:ALA:HB1	6:F:70:VAL:HG11	1.97	0.45
22:a:967:U:H2'	22:a:968:C:C6	2.52	0.45
22:a:2241:A:H2'	22:a:2242:G:C8	2.52	0.45
34:m:56:LYS:HE2	34:m:87:PHE:O	2.16	0.45
39:r:36:LEU:HD13	39:r:48:LYS:HA	1.99	0.45
55:Y:19:G:N2	55:Y:57:G:H1'	2.32	0.45
1:A:728:A:H2'	1:A:729:A:C8	2.52	0.45
1:A:1308:U:H2'	1:A:1309:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:C:O2'	10:J:62:ARG:NH1	2.45	0.45
3:C:186:THR:HG22	3:C:199:LYS:HG2	1.99	0.45
9:I:65:ILE:HD13	9:I:79:ILE:HG23	1.99	0.45
22:a:833:A:H2'	22:a:834:G:C8	2.51	0.45
22:a:1406:U:H2'	22:a:1407:G:H8	1.82	0.45
22:a:2063:C:O2'	55:Y:76:A:O2'	2.27	0.45
22:a:2070:A:H2'	22:a:2071:A:H8	1.82	0.45
27:f:69:LYS:HA	27:f:84:PRO:HA	1.99	0.45
33:l:10:ARG:HE	33:l:11:LYS:HE3	1.81	0.45
42:u:1:MET:SD	42:u:1:MET:N	2.89	0.45
1:A:27:G:H2'	1:A:28:A:C8	2.51	0.45
1:A:236:A:H2'	1:A:237:G:C8	2.52	0.45
1:A:1151:A:O2'	1:A:1152:A:H8	2.00	0.45
4:D:65:TYR:OH	4:D:95:GLU:OE2	2.30	0.45
7:G:68:ASN:O	7:G:138:ARG:NH1	2.44	0.45
7:G:111:ARG:NH1	7:G:123:GLU:OE1	2.49	0.45
11:K:87:LYS:HG3	11:K:115:PRO:HD3	1.98	0.45
16:P:48:GLU:OE1	16:P:51:ARG:NH2	2.40	0.45
22:a:85:G:OP2	41:t:7:ARG:NE	2.50	0.45
22:a:964:C:O2'	22:a:2273:A:N3	2.45	0.45
22:a:2047:C:H2'	22:a:2048:G:H8	1.80	0.45
22:a:2285:C:OP2	48:0:6:ARG:NH1	2.38	0.45
38:q:40:MET:HE2	38:q:49:ILE:HG12	1.98	0.45
1:A:739:C:O2'	15:O:42:HIS:ND1	2.46	0.45
1:A:1350:A:O2'	7:G:33:ASP:OD1	2.34	0.45
1:A:1530:G:H2'	1:A:1531:A:C8	2.52	0.45
22:a:784:G:H5'	22:a:785:G:OP1	2.17	0.45
22:a:1438:U:H2'	22:a:1439:A:C8	2.51	0.45
22:a:1716:U:H2'	22:a:1717:A:C8	2.49	0.45
22:a:2233:U:H2'	22:a:2234:G:H8	1.81	0.45
26:e:5:LEU:HD23	26:e:122:GLU:HB3	1.99	0.45
1:A:321:A:H2'	1:A:322:C:H6	1.81	0.45
1:A:1287:A:N3	1:A:1353:G:O2'	2.44	0.45
1:A:1494:G:O4'	22:a:1913:A:H8	2.00	0.45
4:D:170:TRP:CE2	4:D:186:PRO:HB3	2.52	0.45
6:F:1:MET:HE3	6:F:65:GLU:HG2	1.99	0.45
7:G:53:ARG:HH22	7:G:122:ASN:HA	1.82	0.45
16:P:40:ASN:HB3	16:P:43:ALA:HB2	1.97	0.45
22:a:739:A:H1'	22:a:740:C:H5	1.81	0.45
22:a:2086:U:H2'	22:a:2087:G:H8	1.80	0.45
24:c:62:TYR:HA	24:c:86:ASN:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:z:32:LYS:HE3	47:z:51:GLY:HA3	1.99	0.45
50:2:62:LEU:HB3	50:2:65:ALA:HB2	1.99	0.45
1:A:384:G:H2'	1:A:385:C:H6	1.82	0.45
1:A:512:U:H2'	1:A:513:C:C6	2.52	0.45
1:A:523:A:H61	12:L:89:D2T:H8	1.82	0.45
1:A:1166:G:N1	1:A:1169:A:OP2	2.50	0.45
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.99	0.45
22:a:231:A:H2'	22:a:232:G:O4'	2.17	0.45
22:a:851:C:H2'	22:a:852:U:C6	2.51	0.45
22:a:1198:U:H2'	22:a:1199:U:H6	1.81	0.45
22:a:1363:C:O2'	22:a:1809:A:N3	2.46	0.45
22:a:2233:U:H2'	22:a:2234:G:C8	2.52	0.45
22:a:2566:A:N1	31:j:28:SER:OG	2.37	0.45
22:a:2571:U:O2'	25:d:151:THR:O	2.35	0.45
22:a:2590:A:H2'	22:a:2591:C:H6	1.81	0.45
33:l:53:MET:HE1	33:l:103:TYR:CD1	2.52	0.45
44:w:39:TRP:NE1	44:w:41:GLU:OE1	2.40	0.45
1:A:269:C:H2'	1:A:270:A:H8	1.81	0.44
1:A:1317:C:OP1	14:N:56:SER:OG	2.33	0.44
11:K:97:ILE:HG22	21:U:12:PHE:HZ	1.80	0.44
22:a:2728:U:O2'	22:a:2729:G:H8	1.99	0.44
29:h:8:LYS:HA	29:h:14:SER:HA	1.99	0.44
1:A:427:U:O2'	1:A:541:G:OP1	2.32	0.44
1:A:1219:A:H2'	1:A:1220:G:H8	1.82	0.44
1:A:1330:U:H2'	1:A:1331:G:O4'	2.17	0.44
7:G:18:PHE:HB3	7:G:59:LEU:HD11	1.99	0.44
9:I:11:ARG:HB3	9:I:106:ARG:HH21	1.82	0.44
22:a:634:C:H2'	22:a:635:C:C6	2.52	0.44
22:a:2784:U:H2'	22:a:2785:C:H6	1.83	0.44
30:i:18:VAL:HG21	30:i:142:ILE:HD12	1.99	0.44
1:A:859:G:OP2	1:A:869:G:N1	2.38	0.44
11:K:87:LYS:HB2	11:K:113:VAL:HG23	2.00	0.44
22:a:315:G:H2'	22:a:316:C:C6	2.53	0.44
22:a:519:U:H2'	22:a:520:G:H8	1.82	0.44
22:a:580:U:H2'	22:a:581:C:H6	1.82	0.44
22:a:813:U:H2'	22:a:814:C:C6	2.53	0.44
22:a:876:C:H2'	22:a:877:A:O4'	2.16	0.44
22:a:1183:U:H2'	22:a:1184:U:C6	2.52	0.44
22:a:1316:U:H2'	22:a:1317:G:H8	1.82	0.44
22:a:2266:A:H4'	22:a:2267:A:N3	2.32	0.44
22:a:2461:A:H2'	22:a:2462:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:m:24:MET:HE1	34:m:40:LYS:HD3	1.98	0.44
39:r:46:LEU:O	39:r:50:VAL:HG23	2.17	0.44
1:A:216:U:H2'	1:A:217:C:H6	1.82	0.44
1:A:350:G:H2'	1:A:351:G:C8	2.53	0.44
1:A:709:U:H2'	1:A:710:G:H8	1.82	0.44
8:H:29:SER:HB3	8:H:57:PRO:HB2	2.00	0.44
22:a:909:A:H2'	22:a:912:C:H5	1.81	0.44
22:a:1316:U:H2'	22:a:1317:G:C8	2.52	0.44
22:a:1747:U:H2'	22:a:1748:C:C6	2.53	0.44
1:A:821:G:H2'	1:A:822:U:C6	2.52	0.44
1:A:982:U:H4'	1:A:983:A:O4'	2.17	0.44
1:A:993:G:O2'	1:A:994:A:N7	2.48	0.44
22:a:139:U:H5''	22:a:140:C:H5	1.82	0.44
22:a:191:A:H2'	22:a:192:C:C6	2.52	0.44
22:a:741:U:H2'	22:a:742:A:C8	2.53	0.44
22:a:1527:G:N1	22:a:1544:A:OP2	2.46	0.44
26:e:145:ASP:HB3	26:e:184:ASP:HB2	2.00	0.44
27:f:116:GLY:HA3	27:f:178:ARG:HB3	1.99	0.44
55:Y:15:G:H22	55:Y:48:C:N4	2.16	0.44
1:A:189:A:H8	1:A:189:A:OP2	2.01	0.44
1:A:521:G:N7	12:L:50:ARG:NH1	2.57	0.44
1:A:1401:G:H2'	1:A:1402:4OC:O4'	2.16	0.44
22:a:171:U:H2'	22:a:172:A:C8	2.52	0.44
22:a:966:G:H2'	22:a:967:U:C6	2.53	0.44
22:a:972:A:OP2	22:a:973:A:O2'	2.35	0.44
22:a:1340:U:OP1	40:s:19:LYS:NZ	2.39	0.44
22:a:1812:U:H2'	22:a:1813:G:H8	1.83	0.44
22:a:1949:G:H2'	22:a:1950:G:C8	2.53	0.44
1:A:539:A:H2'	1:A:540:G:H8	1.82	0.44
4:D:19:LEU:HB2	4:D:21:LEU:HG	2.00	0.44
22:a:279:A:C2	22:a:362:A:H5'	2.52	0.44
22:a:632:A:H2'	22:a:633:A:C8	2.52	0.44
22:a:2079:U:O2'	44:w:23:ASN:OD1	2.34	0.44
1:A:191:G:H2'	1:A:192:A:C8	2.52	0.44
1:A:563:A:H2'	1:A:567:G:C8	2.52	0.44
22:a:729:G:O2'	22:a:763:G:H4'	2.17	0.44
22:a:1196:C:C2	22:a:1197:G:C8	3.05	0.44
22:a:2273:A:H2'	22:a:2274:A:C8	2.53	0.44
23:b:39:A:H2'	23:b:40:U:C6	2.53	0.44
35:n:27:VAL:HA	35:n:93:ASP:HB3	2.00	0.44
55:Y:22:G:H2'	55:Y:23:A:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:G:H5''	17:Q:71:LYS:HD3	2.00	0.44
1:A:958:A:C2	19:S:55:ARG:HB3	2.53	0.44
1:A:985:C:H2'	1:A:986:U:C6	2.53	0.44
1:A:1143:G:H2'	1:A:1144:G:C8	2.53	0.44
22:a:306:U:H2'	22:a:307:G:O4'	2.18	0.44
22:a:324:A:N6	22:a:339:U:O4'	2.51	0.44
22:a:871:U:H2'	22:a:872:U:C6	2.53	0.44
22:a:1168:G:H2'	22:a:1169:A:H8	1.82	0.44
22:a:1405:U:H2'	22:a:1406:U:C6	2.52	0.44
22:a:2821:A:OP2	25:d:115:GLY:N	2.48	0.44
46:y:31:ARG:HG2	46:y:34:HIS:HB2	1.99	0.44
1:A:6:G:H4'	1:A:298:A:H4'	1.99	0.43
1:A:1095:U:H2'	1:A:1096:C:H6	1.83	0.43
1:A:1175:G:H2'	1:A:1176:A:C8	2.49	0.43
22:a:296:U:H2'	22:a:297:G:H8	1.83	0.43
22:a:1383:A:H2'	22:a:1384:A:C8	2.53	0.43
22:a:2081:U:H2'	22:a:2082:A:C8	2.53	0.43
23:b:36:C:HO2'	23:b:37:C:P	2.40	0.43
23:b:60:C:H2'	23:b:61:G:C8	2.53	0.43
34:m:79:LEU:HD23	34:m:83:LEU:HD12	2.00	0.43
1:A:35:G:H2'	1:A:36:C:C6	2.52	0.43
1:A:119:A:H5''	1:A:120:A:O4'	2.17	0.43
1:A:294:U:H2'	1:A:295:C:H6	1.83	0.43
1:A:1002:G:H2'	1:A:1003:G:O4'	2.18	0.43
1:A:1180:A:P	9:I:99:ARG:HH12	2.41	0.43
16:P:60:TRP:HA	16:P:63:GLN:HG2	2.00	0.43
22:a:6:A:H2'	22:a:7:G:C8	2.53	0.43
22:a:760:G:H2'	22:a:761:A:O4'	2.18	0.43
22:a:1528:A:H2'	22:a:1529:G:O4'	2.17	0.43
22:a:1738:G:HO2'	22:a:1739:A:H8	1.63	0.43
22:a:2804:U:H2'	22:a:2805:C:C6	2.53	0.43
23:b:5:U:H2'	23:b:6:G:H8	1.82	0.43
31:j:38:ILE:HD11	31:j:112:PHE:HZ	1.83	0.43
1:A:1009:U:H3	1:A:1020:G:H1	1.66	0.43
14:N:20:TYR:HB2	14:N:55:SER:HB2	1.99	0.43
22:a:414:C:H2'	22:a:415:A:C8	2.53	0.43
22:a:667:U:H2'	22:a:668:A:O4'	2.19	0.43
22:a:851:C:H2'	22:a:852:U:H6	1.84	0.43
22:a:1572:A:H2'	22:a:1573:G:H8	1.83	0.43
23:b:40:U:N3	23:b:44:G:OP2	2.35	0.43
24:c:210:ALA:HA	24:c:213:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Y:43:G:H2'	55:Y:44:G:C8	2.54	0.43
1:A:3:A:H5''	1:A:4:U:O4'	2.18	0.43
1:A:21:G:H2'	1:A:22:G:C8	2.54	0.43
1:A:911:U:H2'	1:A:912:C:C6	2.53	0.43
1:A:917:G:H2'	1:A:918:A:C8	2.53	0.43
1:A:1125:U:O2'	1:A:1126:U:O5'	2.26	0.43
1:A:1225:A:H2'	1:A:1225:A:N3	2.33	0.43
22:a:1281:G:H2'	22:a:1282:U:C6	2.53	0.43
22:a:1857:G:N2	22:a:1884:G:N3	2.66	0.43
22:a:2327:A:H2'	22:a:2328:A:C8	2.53	0.43
24:c:16:VAL:HG22	24:c:206:GLY:HA3	1.99	0.43
35:n:6:ALA:O	35:n:10:ARG:HG3	2.19	0.43
1:A:34:C:H2'	1:A:35:G:C8	2.52	0.43
1:A:1035:A:H2'	1:A:1036:A:C8	2.52	0.43
1:A:1343:G:H4'	9:I:124:ARG:HB3	2.01	0.43
2:B:66:LYS:HE3	2:B:158:PRO:HA	2.01	0.43
7:G:140:ASP:HA	7:G:143:ARG:HG2	1.99	0.43
22:a:67:U:C2	22:a:68:G:C8	3.07	0.43
22:a:875:G:H2'	22:a:876:C:C6	2.54	0.43
22:a:1387:A:H2'	22:a:1388:G:C8	2.54	0.43
22:a:1432:G:H2'	22:a:1433:A:H8	1.83	0.43
22:a:2896:C:H2'	22:a:2897:U:C6	2.54	0.43
28:g:137:ASP:HB3	28:g:140:VAL:HB	2.01	0.43
32:k:109:LYS:HE2	32:k:128:THR:HG22	2.01	0.43
34:m:28:LEU:HD23	34:m:48:VAL:HG21	1.99	0.43
46:y:41:THR:HG22	46:y:43:ALA:H	1.83	0.43
1:A:1119:C:H2'	1:A:1120:C:H6	1.84	0.43
10:J:15:HIS:CE1	10:J:16:ARG:HG3	2.53	0.43
22:a:1198:U:C2	22:a:1199:U:C5	3.06	0.43
41:t:36:VAL:HB	41:t:39:ILE:HB	2.01	0.43
55:Y:55:U:O2'	55:Y:57:G:N7	2.42	0.43
1:A:294:U:H2'	1:A:295:C:C6	2.54	0.43
1:A:384:G:H2'	1:A:385:C:C6	2.54	0.43
1:A:460:A:H2'	1:A:461:A:C8	2.54	0.43
1:A:559:A:H4'	1:A:560:A:H3'	2.01	0.43
3:C:134:MET:HE2	3:C:168:TYR:HD2	1.84	0.43
9:I:55:VAL:HG11	9:I:87:LEU:HD13	2.01	0.43
22:a:372:G:OP2	44:w:62:LYS:HE3	2.18	0.43
22:a:644:A:H2'	22:a:645:C:O4'	2.19	0.43
22:a:743:A:O2'	22:a:1659:G:OP1	2.37	0.43
22:a:1049:C:C2	22:a:1050:A:C8	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:40:U:H1'	23:b:45:A:H61	1.83	0.43
26:e:27:LEU:HD11	26:e:100:MET:HB3	1.99	0.43
48:0:13:SER:HB2	48:0:49:TYR:CZ	2.53	0.43
1:A:215:C:H2'	1:A:216:U:H6	1.83	0.43
1:A:1125:U:HO2'	1:A:1126:U:P	2.42	0.43
13:M:84:GLY:HA2	13:M:92:ARG:NH2	2.34	0.43
22:a:17:G:H2'	22:a:18:U:C6	2.54	0.43
22:a:364:C:H2'	22:a:365:U:C6	2.54	0.43
22:a:645:C:H2'	22:a:647:G:N7	2.34	0.43
22:a:682:G:H5'	49:1:26:ASN:CG	2.44	0.43
22:a:1722:A:N6	22:a:1738:G:HO2'	2.16	0.43
22:a:1883:U:H2'	22:a:1884:G:O4'	2.19	0.43
22:a:2216:G:H2'	22:a:2217:G:C8	2.53	0.43
34:m:8:ARG:HD2	34:m:43:GLU:HG2	2.00	0.43
48:0:23:THR:OG1	48:0:24:THR:N	2.51	0.43
55:Y:29:U:H2'	55:Y:30:G:H8	1.83	0.43
1:A:64:G:H4'	1:A:65:A:H3'	1.99	0.43
1:A:575:G:O2'	1:A:821:G:OP2	2.31	0.43
1:A:600:A:H2'	1:A:601:G:C8	2.53	0.43
1:A:867:G:O2'	1:A:873:A:N1	2.50	0.43
8:H:96:MET:SD	8:H:130:ALA:HB1	2.59	0.43
22:a:145:C:H2'	22:a:146:A:C8	2.54	0.43
22:a:721:A:H2'	22:a:722:A:C8	2.54	0.43
22:a:1532:A:C6	22:a:1540:G:C6	3.07	0.43
22:a:2543:G:H2'	22:a:2544:G:C8	2.53	0.43
43:v:37:ILE:HG21	43:v:80:ILE:HG21	2.01	0.43
1:A:920:U:H2'	1:A:921:U:C6	2.54	0.43
1:A:978:A:C4	1:A:1319:A:C2	3.07	0.43
12:L:50:ARG:HG3	12:L:90:LEU:HD21	2.00	0.43
15:O:67:LEU:HD11	15:O:87:LEU:HD13	2.00	0.43
22:a:638:G:H2'	22:a:639:U:C6	2.53	0.43
22:a:1295:C:C2	22:a:1296:G:C8	3.06	0.43
22:a:1417:C:O2'	22:a:1587:G:O2'	2.19	0.43
22:a:1446:C:H2'	22:a:1447:C:C6	2.54	0.43
22:a:1809:A:H2'	22:a:1810:A:C8	2.54	0.43
26:e:146:VAL:HG13	26:e:167:VAL:HG13	2.01	0.43
1:A:67:C:H2'	1:A:68:G:C8	2.54	0.42
1:A:458:U:H2'	1:A:459:A:C8	2.55	0.42
2:B:43:LEU:HA	2:B:46:THR:HB	2.01	0.42
4:D:58:LYS:HD3	4:D:203:LEU:HD23	2.01	0.42
9:I:85:ARG:HA	9:I:88:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:106:ARG:NH1	9:I:107:ASP:O	2.52	0.42
22:a:347:A:H2'	22:a:348:A:C8	2.54	0.42
22:a:358:U:C2	22:a:359:G:C8	3.07	0.42
22:a:1275:A:OP2	22:a:1646:C:N4	2.50	0.42
22:a:1278:C:H2'	22:a:1279:G:C8	2.53	0.42
22:a:1571:A:H2'	22:a:1572:A:H8	1.84	0.42
22:a:1799:G:OP1	24:c:258:ARG:NH1	2.45	0.42
22:a:1812:U:H2'	22:a:1813:G:C8	2.54	0.42
22:a:2311:A:H1'	27:f:85:ILE:HD12	2.00	0.42
25:d:48:ILE:HG23	25:d:84:LEU:HD11	2.01	0.42
55:Y:23:A:H2'	55:Y:24:A:H8	1.84	0.42
1:A:407:U:H2'	1:A:408:A:H8	1.83	0.42
1:A:601:G:H2'	1:A:602:A:H8	1.84	0.42
1:A:745:G:O2'	1:A:746:A:H5'	2.19	0.42
1:A:779:C:H2'	1:A:780:A:O4'	2.19	0.42
1:A:1437:A:H2'	1:A:1438:G:H8	1.83	0.42
22:a:2193:G:H2'	22:a:2194:U:H6	1.84	0.42
22:a:2895:G:H2'	22:a:2896:C:C6	2.55	0.42
41:t:81:ASP:OD1	41:t:82:ARG:N	2.51	0.42
1:A:821:G:H2'	1:A:822:U:H6	1.85	0.42
1:A:1019:A:H2'	1:A:1020:G:O4'	2.20	0.42
1:A:1236:A:H4'	1:A:1304:G:H4'	2.01	0.42
22:a:184:C:H2'	22:a:185:G:C8	2.54	0.42
22:a:438:G:H2'	22:a:439:A:C8	2.54	0.42
22:a:805:G:N2	22:a:829:A:OP1	2.52	0.42
22:a:987:C:H2'	22:a:988:A:O4'	2.19	0.42
22:a:2589:A:H2'	22:a:2590:A:C8	2.54	0.42
1:A:202:G:H2'	1:A:203:G:C8	2.54	0.42
1:A:613:C:H2'	1:A:614:C:C6	2.54	0.42
22:a:40:U:H2'	22:a:41:C:C6	2.54	0.42
22:a:146:A:H2'	22:a:147:C:C6	2.55	0.42
22:a:1113:U:H2'	22:a:1114:C:C6	2.54	0.42
22:a:1737:G:O5'	22:a:1737:G:H8	2.01	0.42
22:a:1799:G:O2'	24:c:180:GLU:OE2	2.32	0.42
22:a:1902:C:H4'	24:c:242:LYS:O	2.20	0.42
22:a:2625:G:H2'	22:a:2626:C:C6	2.54	0.42
1:A:297:G:N2	1:A:300:A:OP2	2.36	0.42
2:B:217:VAL:HA	2:B:220:THR:HG22	2.02	0.42
21:U:51:SER:O	21:U:55:ARG:HG3	2.20	0.42
22:a:52:A:H2'	22:a:53:A:C8	2.55	0.42
22:a:700:G:O2'	22:a:1632:A:N3	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:874:G:H2'	22:a:875:G:H8	1.85	0.42
22:a:1987:A:H2'	22:a:1988:G:H8	1.85	0.42
22:a:2853:C:H2'	22:a:2854:G:H8	1.84	0.42
42:u:2:PHE:CZ	42:u:50:MET:HE2	2.55	0.42
42:u:63:ILE:HG22	42:u:65:VAL:HG23	2.00	0.42
1:A:437:U:O2'	4:D:120:HIS:ND1	2.41	0.42
1:A:634:C:H2'	1:A:635:A:C8	2.55	0.42
1:A:1488:G:H2'	1:A:1489:G:C8	2.55	0.42
2:B:61:ALA:HB3	2:B:224:GLY:HA3	2.02	0.42
9:I:19:VAL:HG22	9:I:65:ILE:HG23	2.02	0.42
22:a:78:U:H2'	22:a:79:C:C6	2.55	0.42
22:a:241:A:N1	22:a:255:A:H5''	2.34	0.42
22:a:1229:C:H2'	22:a:1230:A:C8	2.54	0.42
22:a:1993:U:H4'	25:d:133:THR:OG1	2.20	0.42
1:A:358:U:H2'	1:A:359:G:C8	2.54	0.42
1:A:455:G:H2'	1:A:456:A:H8	1.85	0.42
1:A:580:C:H2'	1:A:581:G:O4'	2.19	0.42
1:A:908:A:H2'	1:A:909:A:C8	2.55	0.42
1:A:966:2MG:N2	55:Y:34:G:H5'	2.34	0.42
1:A:1088:G:H2'	1:A:1089:G:O4'	2.20	0.42
1:A:1320:C:H2'	1:A:1321:U:C6	2.54	0.42
22:a:145:C:H2'	22:a:146:A:H8	1.85	0.42
22:a:414:C:H2'	22:a:415:A:H8	1.85	0.42
22:a:562:U:H1'	22:a:2035:G:O2'	2.20	0.42
30:i:141:ASP:OD1	30:i:141:ASP:N	2.51	0.42
45:x:9:LYS:HB3	45:x:13:GLU:HB2	2.00	0.42
1:A:132:C:H4'	1:A:262:A:H1'	2.01	0.42
1:A:513:C:H2'	1:A:514:C:H6	1.85	0.42
1:A:1463:U:H2'	1:A:1464:U:C6	2.55	0.42
2:B:71:GLY:O	2:B:93:ASN:HA	2.20	0.42
4:D:139:PRO:HA	4:D:182:PHE:HD2	1.84	0.42
11:K:79:ILE:HB	11:K:105:PHE:HE1	1.84	0.42
15:O:25:THR:HG21	15:O:70:LEU:HB2	2.01	0.42
22:a:697:G:H2'	22:a:698:C:C6	2.55	0.42
22:a:710:U:H2'	22:a:711:G:H8	1.85	0.42
22:a:1726:C:H2'	22:a:1727:C:H6	1.84	0.42
22:a:2639:A:H2'	22:a:2640:G:O4'	2.20	0.42
22:a:2683:C:H5''	36:o:56:HIS:HB3	2.02	0.42
22:a:2785:C:H2'	22:a:2786:U:H6	1.85	0.42
23:b:40:U:H2'	52:4:2:LYS:HE3	2.00	0.42
3:C:16:LYS:NZ	3:C:181:ASP:OD1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:742:A:H2'	22:a:743:A:H8	1.84	0.42
22:a:1197:G:H2'	22:a:1198:U:H6	1.84	0.42
22:a:1747:U:H2'	22:a:1748:C:H6	1.85	0.42
22:a:2377:A:H2'	22:a:2378:A:C8	2.55	0.42
22:a:2636:C:H2'	22:a:2637:U:C6	2.55	0.42
26:e:176:ASP:OD1	26:e:176:ASP:N	2.51	0.42
42:u:4:ILE:HG12	42:u:50:MET:HE1	2.02	0.42
1:A:799:G:H2'	1:A:800:G:O4'	2.20	0.42
2:B:187:VAL:HG13	2:B:191:SER:HB3	2.02	0.42
3:C:36:ASP:OD1	3:C:59:ARG:NH2	2.47	0.42
3:C:77:ILE:HA	3:C:84:VAL:HG13	2.02	0.42
22:a:577:G:O2'	22:a:1254:A:OP1	2.36	0.42
22:a:885:C:H2'	22:a:886:A:O4'	2.20	0.42
22:a:1721:G:N2	22:a:1738:G:H2'	2.35	0.42
22:a:1771:C:H2'	22:a:1772:A:C8	2.55	0.42
22:a:2590:A:H2'	22:a:2591:C:C6	2.55	0.42
22:a:2680:U:H2'	22:a:2681:C:C6	2.55	0.42
40:s:34:VAL:HG21	40:s:43:ILE:HD11	2.01	0.42
1:A:33:A:H2'	1:A:34:C:C6	2.55	0.41
1:A:315:A:O2'	1:A:330:C:O2'	2.32	0.41
1:A:766:A:OP2	1:A:812:G:N2	2.53	0.41
1:A:918:A:H2'	1:A:919:A:C8	2.55	0.41
1:A:982:U:H5''	14:N:6:MET:HE3	2.02	0.41
1:A:1493:A:O2'	22:a:1913:A:N7	2.45	0.41
6:F:40:GLU:OE1	6:F:100:SER:OG	2.24	0.41
22:a:566:U:H5''	32:k:29:LYS:HE3	2.02	0.41
22:a:741:U:H2'	22:a:742:A:H8	1.85	0.41
22:a:1224:U:H2'	22:a:1225:G:C8	2.55	0.41
22:a:2547:A:H4'	31:j:29:HIS:CE1	2.55	0.41
55:Y:10:G:N1	55:Y:26:A:H1'	2.35	0.41
1:A:399:G:H2'	1:A:400:C:C6	2.55	0.41
1:A:494:G:O2'	1:A:496:A:H1'	2.20	0.41
1:A:768:A:H4'	1:A:1523:G:N2	2.35	0.41
1:A:1130:A:C8	1:A:1146:A:C2	3.08	0.41
7:G:111:ARG:HD3	7:G:119:ARG:O	2.21	0.41
18:R:23:TYR:HA	18:R:29:LEU:HD11	2.03	0.41
22:a:597:G:N2	32:k:12:SER:O	2.50	0.41
22:a:680:C:H2'	22:a:681:G:C8	2.55	0.41
22:a:1038:G:H2'	22:a:1039:A:C8	2.55	0.41
22:a:2698:U:H2'	22:a:2699:C:H6	1.86	0.41
40:s:2:ILE:HD13	40:s:42:GLU:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:6:GLN:O	44:w:74:ARG:NH1	2.50	0.41
1:A:590:U:OP1	8:H:31:LYS:HG2	2.20	0.41
1:A:1147:C:H2'	1:A:1148:U:C6	2.56	0.41
2:B:164:ILE:O	2:B:186:ILE:HB	2.20	0.41
4:D:27:ALA:O	4:D:30:THR:OG1	2.36	0.41
9:I:55:VAL:HG23	9:I:57:MET:H	1.85	0.41
11:K:81:ASN:OD1	11:K:81:ASN:N	2.54	0.41
22:a:150:U:H2'	22:a:151:C:C6	2.54	0.41
22:a:399:U:O4	44:w:54:LYS:NZ	2.53	0.41
22:a:858:G:OP1	43:v:78:LYS:NZ	2.43	0.41
23:b:49:C:H2'	23:b:50:A:C8	2.54	0.41
31:j:77:ILE:HG12	36:o:72:ARG:HG3	2.03	0.41
1:A:20:U:H2'	1:A:21:G:O4'	2.19	0.41
1:A:500:G:H2'	1:A:501:C:C6	2.55	0.41
1:A:1062:U:H2'	1:A:1063:C:C6	2.56	0.41
1:A:1494:G:H1'	22:a:1913:A:H5'	2.01	0.41
7:G:5:ARG:HD2	7:G:5:ARG:HA	1.91	0.41
11:K:19:GLY:O	11:K:37:ARG:NH1	2.53	0.41
22:a:151:C:H2'	22:a:152:A:C8	2.54	0.41
22:a:959:A:H2'	22:a:960:A:C8	2.55	0.41
22:a:1325:U:C4	59:a:6197:SPD:H52	2.55	0.41
22:a:2467:C:O2	33:l:123:LYS:NZ	2.47	0.41
22:a:2758:A:C2	28:g:71:LEU:HD11	2.54	0.41
22:a:2804:U:H2'	22:a:2805:C:H6	1.85	0.41
22:a:2819:G:H2'	22:a:2821:A:N7	2.36	0.41
29:h:30:LEU:HB3	29:h:36:ALA:HB3	2.02	0.41
42:u:6:ALA:HB1	42:u:40:ILE:HB	2.02	0.41
46:y:47:MET:O	46:y:51:VAL:HG22	2.20	0.41
1:A:255:G:H4'	17:Q:19:LYS:HD2	2.01	0.41
1:A:470:C:H2'	1:A:471:U:C6	2.55	0.41
1:A:472:U:H2'	1:A:473:U:H6	1.86	0.41
1:A:473:U:C2	1:A:474:G:C8	3.09	0.41
1:A:537:G:H5''	12:L:110:ARG:NH1	2.36	0.41
1:A:883:C:H2'	1:A:884:U:C6	2.55	0.41
1:A:1032:G:H3'	1:A:1032:G:N3	2.36	0.41
1:A:1090:U:H2'	1:A:1091:U:C6	2.54	0.41
1:A:1355:G:H2'	1:A:1356:G:H8	1.84	0.41
22:a:261:G:C2	22:a:262:A:C8	3.08	0.41
22:a:264:C:H4'	22:a:265:A:OP1	2.20	0.41
22:a:813:U:H2'	22:a:814:C:H6	1.85	0.41
22:a:1286:A:H1'	22:a:1288:G:OP2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1327:A:H2'	22:a:1328:A:O4'	2.21	0.41
22:a:1395:A:O2'	22:a:1396:U:H5''	2.20	0.41
22:a:1440:U:H2'	22:a:1441:G:C8	2.55	0.41
22:a:1594:U:H2'	22:a:1595:C:C6	2.55	0.41
22:a:1889:A:H2'	22:a:1890:A:C8	2.55	0.41
22:a:1992:G:N2	22:a:1996:C:O2'	2.53	0.41
32:k:78:ARG:HG2	32:k:113:ALA:HB3	2.03	0.41
55:Y:58:A:O2'	55:Y:60:U:OP2	2.35	0.41
1:A:215:C:H2'	1:A:216:U:C6	2.56	0.41
1:A:876:C:H2'	1:A:877:G:H8	1.86	0.41
1:A:1152:A:P	10:J:72:ARG:HH22	2.43	0.41
1:A:1217:C:P	14:N:9:ARG:HH21	2.42	0.41
1:A:1300:G:H1'	1:A:1303:C:N4	2.35	0.41
1:A:1477:U:H2'	1:A:1478:U:C6	2.56	0.41
22:a:1013:C:H2'	22:a:1014:A:C8	2.56	0.41
22:a:1294:U:O2	34:m:23:ASN:ND2	2.54	0.41
22:a:1571:A:H2'	22:a:1572:A:C8	2.56	0.41
22:a:2637:U:H5''	25:d:83:ARG:HH21	1.85	0.41
23:b:66:A:N6	23:b:107:G:H2'	2.35	0.41
23:b:104:A:H2'	23:b:105:G:O4'	2.21	0.41
36:o:9:GLU:O	36:o:13:MET:HG3	2.21	0.41
1:A:69:G:H2'	1:A:70:U:C6	2.55	0.41
1:A:214:C:H2'	1:A:215:C:C6	2.56	0.41
1:A:1100:C:H3'	2:B:95:ARG:HH21	1.86	0.41
2:B:159:ASP:O	2:B:182:PRO:HD2	2.20	0.41
12:L:110:ARG:HH21	12:L:113:ALA:HB3	1.86	0.41
22:a:1115:G:O2'	22:a:1116:G:OP1	2.38	0.41
22:a:1509:A:H2'	22:a:1510:G:C8	2.56	0.41
22:a:1664:A:H61	22:a:1996:C:N4	2.18	0.41
22:a:2051:A:H8	22:a:2051:A:OP2	2.03	0.41
22:a:2097:A:H2'	22:a:2098:U:C6	2.55	0.41
22:a:2700:A:H2'	22:a:2701:U:C6	2.56	0.41
38:q:5:PHE:HB3	38:q:59:ILE:HD12	2.03	0.41
1:A:224:U:H2'	1:A:225:C:C6	2.56	0.41
1:A:923:A:H2'	1:A:924:C:C6	2.55	0.41
1:A:967:5MC:OP2	1:A:968:A:O2'	2.32	0.41
1:A:1170:A:H2'	1:A:1171:A:O4'	2.20	0.41
7:G:65:ALA:O	7:G:69:VAL:HG23	2.20	0.41
7:G:88:PRO:HG3	7:G:149:LYS:HA	2.03	0.41
22:a:307:G:N1	22:a:310:A:OP2	2.42	0.41
22:a:858:G:N3	22:a:2268:A:H2'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1130:U:C2	22:a:2025:C:H5''	2.56	0.41
22:a:1440:U:H2'	22:a:1441:G:H8	1.86	0.41
22:a:1710:G:H2'	22:a:1711:A:C8	2.56	0.41
31:j:9:ASN:O	31:j:83:ALA:HA	2.21	0.41
33:l:17:ASN:OD1	33:l:97:GLN:NE2	2.54	0.41
33:l:56:ALA:HB2	33:l:119:LEU:HD12	2.03	0.41
43:v:17:GLU:O	43:v:19:LYS:NZ	2.53	0.41
1:A:126:G:OP1	1:A:605:U:O2'	2.28	0.41
1:A:161:A:H2'	1:A:162:A:C8	2.56	0.41
1:A:255:G:H2'	1:A:256:U:C6	2.56	0.41
1:A:269:C:H2'	1:A:270:A:C8	2.56	0.41
1:A:321:A:H2'	1:A:322:C:C6	2.55	0.41
1:A:337:G:C2	1:A:338:A:C5	3.08	0.41
1:A:515:G:H2'	1:A:516:PSU:H6	1.86	0.41
1:A:721:G:H4'	1:A:722:G:O4'	2.21	0.41
1:A:751:U:H2'	1:A:752:G:O4'	2.20	0.41
1:A:1014:A:C2	1:A:1219:A:H1'	2.55	0.41
1:A:1107:C:C4	1:A:1108:G:C8	3.09	0.41
3:C:47:LEU:HB3	3:C:50:ALA:HB3	2.01	0.41
3:C:58:GLU:OE1	3:C:65:ARG:NH2	2.54	0.41
10:J:11:LYS:HG2	10:J:71:LEU:HD13	2.03	0.41
11:K:34:ILE:HB	11:K:74:VAL:HG11	2.01	0.41
14:N:53:ARG:HB3	14:N:59:ARG:NH1	2.36	0.41
20:T:67:ILE:HB	20:T:71:LYS:HD3	2.02	0.41
20:T:68:HIS:CD2	20:T:70:ASN:H	2.39	0.41
22:a:18:U:O2'	22:a:554:U:OP1	2.39	0.41
22:a:513:A:H5''	22:a:1216:G:O2'	2.21	0.41
22:a:591:U:H1'	50:2:2:PRO:HD2	2.03	0.41
22:a:675:A:OP1	26:e:58:LYS:NZ	2.41	0.41
22:a:769:U:C2	22:a:770:G:C8	3.09	0.41
22:a:817:C:O2'	22:a:839:U:H5''	2.21	0.41
22:a:918:A:N3	23:b:80:U:O2'	2.49	0.41
22:a:1036:G:C6	22:a:1120:G:C6	3.09	0.41
22:a:1113:U:H2'	22:a:1114:C:H6	1.86	0.41
22:a:1387:A:H2'	22:a:1388:G:H8	1.84	0.41
22:a:1412:U:H2'	22:a:1413:A:H8	1.86	0.41
22:a:1710:G:H4'	22:a:2858:C:O2	2.21	0.41
23:b:16:G:N2	23:b:69:G:H1'	2.36	0.41
26:e:173:THR:HA	26:e:199:MET:HE1	2.02	0.41
26:e:196:VAL:HA	26:e:199:MET:HG2	2.03	0.41
32:k:2:ARG:H	32:k:5:THR:HG1	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:79:LEU:HD11	32:k:112:LEU:HD12	2.03	0.41
43:v:25:ARG:HH11	43:v:31:VAL:HG12	1.85	0.41
45:x:39:GLN:HB3	45:x:41:HIS:CE1	2.56	0.41
1:A:70:U:O2'	1:A:94:G:N7	2.49	0.41
1:A:309:A:H2'	1:A:310:G:H8	1.86	0.41
1:A:1060:U:OP1	14:N:85:ARG:NH2	2.52	0.41
1:A:1355:G:H2'	1:A:1356:G:C8	2.56	0.41
5:E:14:LYS:NZ	5:E:116:GLU:HG2	2.36	0.41
20:T:28:MET:HE2	20:T:28:MET:HB3	1.98	0.41
22:a:44:A:H2'	22:a:45:G:O4'	2.20	0.41
22:a:476:G:N1	22:a:479:A:OP2	2.44	0.41
22:a:577:G:H2'	22:a:578:G:C8	2.56	0.41
22:a:745:1MG:O2'	22:a:748:G:H1'	2.21	0.41
22:a:796:C:H2'	22:a:797:G:C8	2.55	0.41
22:a:1009:A:N3	22:a:1153:C:O2'	2.52	0.41
24:c:168:ASP:OD1	24:c:168:ASP:N	2.54	0.41
25:d:131:ASP:O	25:d:136:ASN:ND2	2.45	0.41
27:f:38:MET:HB2	27:f:87:CYS:SG	2.61	0.41
29:h:54:LEU:O	29:h:57:LYS:HG2	2.21	0.41
41:t:86:ARG:HG3	41:t:95:PHE:CE1	2.56	0.41
55:Y:62:C:H2'	55:Y:63:C:C6	2.56	0.41
1:A:1010:U:H2'	1:A:1011:C:O4'	2.22	0.40
1:A:1241:G:H2'	1:A:1242:G:H8	1.86	0.40
11:K:18:ASP:HB2	11:K:37:ARG:NH2	2.36	0.40
22:a:12:U:O2	22:a:2626:C:H4'	2.21	0.40
22:a:287:G:H2'	22:a:288:U:C6	2.56	0.40
22:a:1874:C:H2'	22:a:1875:G:O4'	2.21	0.40
22:a:2251:OMG:H1'	22:a:2251:OMG:HM23	1.78	0.40
23:b:1:U:H2'	23:b:2:G:C8	2.55	0.40
23:b:106:G:H2'	23:b:107:G:O4'	2.21	0.40
24:c:61:ALA:O	24:c:63:ARG:NH1	2.54	0.40
35:n:115:LEU:HD23	35:n:115:LEU:HA	1.91	0.40
36:o:51:ARG:CZ	36:o:53:ARG:HG3	2.51	0.40
42:u:5:ASN:HD22	42:u:64:VAL:HB	1.87	0.40
1:A:75:G:C4	1:A:76:G:C8	3.09	0.40
1:A:109:A:H5'	1:A:110:C:C5	2.56	0.40
1:A:217:C:H2'	1:A:218:U:H6	1.87	0.40
1:A:309:A:O2'	1:A:607:A:N1	2.47	0.40
1:A:410:G:H2'	1:A:429:U:C4	2.56	0.40
1:A:545:C:H5'	4:D:69:GLU:HB2	2.02	0.40
1:A:1120:C:H2'	1:A:1121:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:G:H2'	1:A:1531:A:H8	1.87	0.40
6:F:42:TRP:HB2	6:F:59:TYR:HB2	2.04	0.40
9:I:10:GLY:HA3	9:I:78:ALA:O	2.21	0.40
12:L:90:LEU:HA	12:L:91:PRO:HD3	1.96	0.40
22:a:138:U:O2'	22:a:141:G:O6	2.32	0.40
22:a:468:G:N7	49:1:39:ARG:NH2	2.57	0.40
22:a:875:G:H2'	22:a:876:C:H6	1.86	0.40
22:a:1125:G:OP2	22:a:1126:A:O2'	2.29	0.40
22:a:1181:U:H2'	22:a:1182:G:C8	2.56	0.40
22:a:1417:C:H2'	22:a:1418:G:O4'	2.22	0.40
22:a:2623:G:H4'	22:a:2825:G:H8	1.86	0.40
22:a:2747:G:O6	22:a:2755:C:H5''	2.20	0.40
22:a:2748:A:H5'	28:g:4:VAL:HG21	2.03	0.40
24:c:80:ARG:NE	24:c:82:GLU:OE2	2.53	0.40
25:d:12:THR:OG1	25:d:13:ARG:N	2.54	0.40
26:e:51:GLU:OE2	26:e:88:ARG:NH2	2.54	0.40
26:e:171:ASP:OD2	26:e:173:THR:OG1	2.40	0.40
1:A:1095:U:P	1:A:1108:G:H1	2.44	0.40
1:A:1323:G:H2'	1:A:1324:A:C8	2.56	0.40
3:C:117:ALA:HB1	3:C:187:SER:OG	2.21	0.40
10:J:52:LEU:HB2	14:N:81:ARG:HD2	2.03	0.40
13:M:94:GLY:O	13:M:109:ARG:HB3	2.22	0.40
20:T:30:THR:HG22	20:T:34:LYS:HE3	2.02	0.40
22:a:591:U:H2'	22:a:592:A:C8	2.55	0.40
22:a:633:A:O2'	22:a:2404:U:OP1	2.35	0.40
22:a:1298:C:H2'	22:a:1299:G:O4'	2.21	0.40
22:a:1857:G:H1'	22:a:1885:A:N6	2.37	0.40
22:a:2247:A:H2'	22:a:2248:C:H6	1.85	0.40
22:a:2489:U:H2'	22:a:2490:G:O4'	2.20	0.40
24:c:145:GLU:HG2	24:c:151:GLY:C	2.46	0.40
28:g:52:PHE:CZ	28:g:69:ARG:HA	2.57	0.40
41:t:33:LYS:HB3	41:t:64:ALA:HB1	2.04	0.40
1:A:512:U:H2'	1:A:513:C:H6	1.86	0.40
1:A:925:G:C2	1:A:927:G:C8	3.10	0.40
1:A:1447:A:OP1	1:A:1448:C:N4	2.36	0.40
22:a:499:U:H2'	22:a:500:G:O4'	2.21	0.40
22:a:594:U:H2'	22:a:595:C:C6	2.56	0.40
22:a:634:C:H2'	22:a:635:C:H6	1.86	0.40
22:a:724:U:H2'	22:a:725:G:C8	2.57	0.40
22:a:877:A:C6	22:a:899:A:C6	3.09	0.40
22:a:1387:A:H5'	22:a:1469:A:H1'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2030:6MZ:C2	22:a:2499:C:H5''	2.51	0.40
22:a:2062:A:C6	53:W:4:LEU:HD11	2.57	0.40
27:f:6:ASP:HA	27:f:9:LYS:HE2	2.03	0.40
42:u:6:ALA:HB3	42:u:65:VAL:HG22	2.04	0.40
42:u:80:HIS:CG	42:u:81:PRO:HD2	2.57	0.40
1:A:578:C:O2'	1:A:728:A:N3	2.41	0.40
1:A:996:A:H2'	1:A:997:U:C6	2.57	0.40
1:A:1070:U:H2'	1:A:1071:C:C6	2.56	0.40
1:A:1356:G:H2'	1:A:1357:A:H8	1.87	0.40
1:A:1496:C:H2'	1:A:1497:G:O4'	2.22	0.40
3:C:6:HIS:CE1	3:C:8:ASN:HB3	2.57	0.40
3:C:18:TRP:HZ2	14:N:97:LYS:HG2	1.86	0.40
9:I:28:ILE:HD12	9:I:35:LEU:HD22	2.04	0.40
20:T:31:PHE:O	20:T:35:VAL:HG23	2.22	0.40
22:a:278:A:C6	22:a:362:A:C8	3.09	0.40
22:a:820:A:H4'	22:a:836:G:N2	2.32	0.40
22:a:881:G:H2'	22:a:882:G:H8	1.86	0.40
34:m:86:ARG:HH21	34:m:117:ASP:CG	2.29	0.40
42:u:75:GLN:HB2	42:u:92:VAL:HG23	2.02	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	223/241 (92%)	220 (99%)	3 (1%)	0	100	100
3	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
4	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
5	E	154/167 (92%)	153 (99%)	1 (1%)	0	100	100
6	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	151/179 (84%)	149 (99%)	2 (1%)	0	100	100
8	H	127/130 (98%)	127 (100%)	0	0	100	100
9	I	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	J	97/103 (94%)	96 (99%)	1 (1%)	0	100	100
11	K	113/129 (88%)	111 (98%)	2 (2%)	0	100	100
12	L	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	M	114/118 (97%)	110 (96%)	4 (4%)	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%)	75 (95%)	4 (5%)	0	100	100
17	Q	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	R	64/75 (85%)	64 (100%)	0	0	100	100
19	S	82/92 (89%)	82 (100%)	0	0	100	100
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
24	c	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
25	d	206/209 (99%)	203 (98%)	3 (2%)	0	100	100
26	e	199/201 (99%)	199 (100%)	0	0	100	100
27	f	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
28	g	172/177 (97%)	168 (98%)	4 (2%)	0	100	100
29	h	65/149 (44%)	61 (94%)	4 (6%)	0	100	100
30	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
31	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
32	k	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
33	l	132/136 (97%)	132 (100%)	0	0	100	100
34	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
35	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
36	o	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
37	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
38	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
39	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	s	91/100 (91%)	91 (100%)	0	0	100	100
41	t	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
42	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
43	v	76/85 (89%)	76 (100%)	0	0	100	100
44	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
45	x	60/63 (95%)	60 (100%)	0	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	54 (100%)	0	0	100	100
48	0	49/55 (89%)	49 (100%)	0	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
51	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
52	4	45/70 (64%)	45 (100%)	0	0	100	100
53	W	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
All	All	5510/5927 (93%)	5421 (98%)	89 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	185 (100%)	1 (0%)	81	93
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	105/107 (98%)	104 (99%)	1 (1%)	68	89
10	J	87/90 (97%)	87 (100%)	0	100	100
11	K	89/98 (91%)	89 (100%)	0	100	100
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	94/96 (98%)	94 (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	74/78 (95%)	74 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	59 (98%)	1 (2%)	53	82
24	c	216/218 (99%)	216 (100%)	0	100	100
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	135/138 (98%)	135 (100%)	0	100	100
29	h	50/114 (44%)	49 (98%)	1 (2%)	48	78
30	i	116/116 (100%)	116 (100%)	0	100	100
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	107/107 (100%)	107 (100%)	0	100	100
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	86 (100%)	0	100	100
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100
39	r	93/93 (100%)	93 (100%)	0	100	100
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	u	78/78 (100%)	78 (100%)	0	100	100
43	v	59/63 (94%)	59 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	54 (100%)	0	100	100
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100
48	0	46/49 (94%)	46 (100%)	0	100	100
49	1	38/38 (100%)	38 (100%)	0	100	100
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	43/62 (69%)	43 (100%)	0	100	100
53	W	10/10 (100%)	10 (100%)	0	100	100
All	All	4590/4835 (95%)	4586 (100%)	4 (0%)	87	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	151	ILE
9	I	18	ARG
21	U	40	LYS
29	h	37	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	GLN
2	B	42	ASN
2	B	146	ASN
3	C	3	GLN
3	C	100	GLN
3	C	102	ASN
3	C	139	GLN
4	D	40	GLN
4	D	100	ASN
4	D	131	ASN
4	D	136	GLN
4	D	152	GLN

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Mol	Chain	Res	Type
5	E	82	GLN
5	E	148	ASN
6	F	46	GLN
6	F	94	HIS
7	G	52	GLN
7	G	68	ASN
7	G	142	HIS
8	H	118	GLN
9	I	110	GLN
11	K	15	GLN
11	K	38	GLN
11	K	40	ASN
12	L	112	GLN
13	M	14	HIS
14	N	60	GLN
14	N	66	GLN
15	O	35	GLN
15	O	40	GLN
15	O	80	GLN
16	P	63	GLN
17	Q	51	ASN
19	S	57	HIS
20	T	13	GLN
20	T	68	HIS
21	U	64	ASN
24	c	53	HIS
24	c	163	GLN
24	c	260	ASN
25	d	36	GLN
25	d	49	GLN
25	d	140	HIS
25	d	173	GLN
25	d	185	ASN
26	e	115	GLN
26	e	136	GLN
27	f	5	HIS
27	f	27	GLN
28	g	88	GLN
28	g	115	HIS
29	h	18	GLN
29	h	28	ASN
30	i	136	GLN

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Mol	Chain	Res	Type
31	j	3	GLN
32	k	104	GLN
33	l	13	HIS
33	l	60	GLN
35	n	29	HIS
36	o	10	GLN
37	p	20	GLN
37	p	37	GLN
37	p	44	GLN
37	p	52	GLN
37	p	71	GLN
38	q	12	HIS
39	r	40	ASN
40	s	72	GLN
40	s	91	GLN
42	u	5	ASN
42	u	49	ASN
44	w	20	HIS
44	w	36	HIS
45	x	27	ASN
45	x	58	ASN
51	3	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1542 (97%)	194 (12%)	1 (0%)
22	a	2749/2904 (94%)	342 (12%)	0
23	b	118/120 (98%)	12 (10%)	0
54	X	8/9 (88%)	1 (12%)	0
55	Y	70/77 (90%)	12 (17%)	0
56	Z	1/3 (33%)	0	0
All	All	4449/4655 (95%)	561 (12%)	1 (0%)

All (561) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	7	A
1	A	9	G
1	A	22	G

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Mol	Chain	Res	Type
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	68	G
1	A	71	A
1	A	74	A
1	A	75	G
1	A	76	G
1	A	92	U
1	A	95	C
1	A	121	U
1	A	131	A
1	A	138	G
1	A	144	G
1	A	166	U
1	A	181	A
1	A	189	A
1	A	197	A
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	283	U
1	A	289	G
1	A	328	C
1	A	330	C
1	A	344	A
1	A	352	C
1	A	354	G
1	A	355	C
1	A	367	U
1	A	368	U
1	A	369	G
1	A	372	C
1	A	388	G
1	A	392	C
1	A	406	G
1	A	412	A

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Mol	Chain	Res	Type
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	456	A
1	A	457	G
1	A	458	U
1	A	459	A
1	A	463	U
1	A	464	U
1	A	467	U
1	A	468	A
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	491	G
1	A	495	A
1	A	496	A
1	A	497	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	524	G
1	A	530	G
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	564	C
1	A	570	G
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	596	A
1	A	633	G
1	A	650	G

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Mol	Chain	Res	Type
1	A	661	G
1	A	665	A
1	A	687	A
1	A	721	G
1	A	723	U
1	A	734	G
1	A	746	A
1	A	748	G
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	811	C
1	A	815	A
1	A	817	C
1	A	821	G
1	A	832	G
1	A	890	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	993	G
1	A	1003	G
1	A	1004	A
1	A	1007	U
1	A	1020	G
1	A	1024	G
1	A	1028	C
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G

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Mol	Chain	Res	Type
1	A	1035	A
1	A	1036	A
1	A	1039	G
1	A	1042	A
1	A	1044	A
1	A	1065	U
1	A	1085	U
1	A	1089	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1125	U
1	A	1133	G
1	A	1137	C
1	A	1139	G
1	A	1141	C
1	A	1144	G
1	A	1152	A
1	A	1159	U
1	A	1167	A
1	A	1174	G
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1250	A
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1346	A
1	A	1363	A
1	A	1364	U
1	A	1368	A

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Mol	Chain	Res	Type
1	A	1370	G
1	A	1372	U
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1419	G
1	A	1432	G
1	A	1446	A
1	A	1452	C
1	A	1490	U
1	A	1491	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
22	a	10	A
22	a	12	U
22	a	14	A
22	a	27	G
22	a	29	U
22	a	34	U
22	a	35	G
22	a	51	G
22	a	71	A
22	a	74	A
22	a	75	G
22	a	84	A
22	a	101	A
22	a	102	U
22	a	118	A
22	a	120	U
22	a	136	G
22	a	137	U
22	a	139	U
22	a	163	C

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Mol	Chain	Res	Type
22	a	181	A
22	a	196	A
22	a	199	A
22	a	216	A
22	a	222	A
22	a	223	A
22	a	233	A
22	a	248	G
22	a	250	G
22	a	251	A
22	a	265	A
22	a	275	C
22	a	276	U
22	a	280	U
22	a	281	C
22	a	282	A
22	a	284	U
22	a	287	G
22	a	290	U
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	356	G
22	a	361	G
22	a	362	A
22	a	367	G
22	a	386	G
22	a	396	G
22	a	402	A
22	a	404	A
22	a	405	U
22	a	411	G
22	a	412	A
22	a	417	C
22	a	481	G
22	a	491	G
22	a	505	A
22	a	507	A
22	a	509	C
22	a	513	A
22	a	529	A

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Mol	Chain	Res	Type
22	a	530	G
22	a	532	A
22	a	545	U
22	a	546	U
22	a	547	A
22	a	550	C
22	a	563	A
22	a	568	U
22	a	573	U
22	a	575	A
22	a	603	A
22	a	611	C
22	a	614	A
22	a	615	U
22	a	621	A
22	a	627	A
22	a	637	A
22	a	644	A
22	a	645	C
22	a	646	U
22	a	647	G
22	a	655	A
22	a	685	A
22	a	686	U
22	a	717	C
22	a	721	A
22	a	726	G
22	a	730	A
22	a	740	C
22	a	747	5MU
22	a	764	A
22	a	765	C
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	789	A
22	a	805	G
22	a	812	C
22	a	827	U
22	a	829	A

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Mol	Chain	Res	Type
22	a	845	A
22	a	846	U
22	a	859	G
22	a	879	G
22	a	880	G
22	a	881	G
22	a	883	G
22	a	884	U
22	a	888	C
22	a	890	C
22	a	891	G
22	a	892	A
22	a	896	A
22	a	897	C
22	a	899	A
22	a	907	G
22	a	910	A
22	a	914	G
22	a	931	U
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	996	A
22	a	1009	A
22	a	1012	U
22	a	1013	C
22	a	1026	G
22	a	1033	U
22	a	1045	C
22	a	1047	G
22	a	1110	G
22	a	1111	A
22	a	1112	G
22	a	1115	G
22	a	1116	G
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1169	A
22	a	1172	C

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Mol	Chain	Res	Type
22	a	1204	A
22	a	1212	G
22	a	1213	A
22	a	1236	G
22	a	1237	A
22	a	1247	A
22	a	1250	G
22	a	1253	A
22	a	1255	U
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1273	U
22	a	1279	G
22	a	1300	G
22	a	1301	A
22	a	1309	G
22	a	1329	U
22	a	1341	G
22	a	1365	A
22	a	1378	A
22	a	1379	U
22	a	1383	A
22	a	1395	A
22	a	1398	C
22	a	1416	G
22	a	1417	C
22	a	1428	C
22	a	1437	C
22	a	1452	G
22	a	1478	G
22	a	1482	G
22	a	1490	A
22	a	1493	C
22	a	1508	A
22	a	1509	A
22	a	1515	A
22	a	1524	G
22	a	1535	A
22	a	1536	C
22	a	1554	U
22	a	1557	C

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Mol	Chain	Res	Type
22	a	1558	C
22	a	1560	G
22	a	1569	A
22	a	1571	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1608	A
22	a	1610	A
22	a	1626	A
22	a	1634	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1715	G
22	a	1729	U
22	a	1730	C
22	a	1733	G
22	a	1738	G
22	a	1756	G
22	a	1764	C
22	a	1773	A
22	a	1784	A
22	a	1786	A
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1827	U
22	a	1829	A
22	a	1847	A
22	a	1848	A
22	a	1858	A
22	a	1868	C
22	a	1869	G
22	a	1870	C
22	a	1871	A
22	a	1872	A
22	a	1906	G
22	a	1929	G
22	a	1930	G

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Mol	Chain	Res	Type
22	a	1937	A
22	a	1955	U
22	a	1964	G
22	a	1966	A
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1992	G
22	a	1993	U
22	a	2021	C
22	a	2023	C
22	a	2030	6MZ
22	a	2031	A
22	a	2033	A
22	a	2035	G
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2093	G
22	a	2198	A
22	a	2204	G
22	a	2211	A
22	a	2225	A
22	a	2238	G
22	a	2239	G
22	a	2271	G
22	a	2278	A
22	a	2283	C
22	a	2287	A
22	a	2288	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2345	G

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Mol	Chain	Res	Type
22	a	2347	C
22	a	2361	G
22	a	2383	G
22	a	2385	C
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2422	C
22	a	2429	G
22	a	2430	A
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2469	A
22	a	2470	G
22	a	2475	C
22	a	2476	A
22	a	2491	U
22	a	2494	G
22	a	2498	OMC
22	a	2502	G
22	a	2504	PSU
22	a	2505	G
22	a	2506	U
22	a	2518	A
22	a	2520	C
22	a	2529	G
22	a	2547	A
22	a	2566	A
22	a	2567	G
22	a	2572	A
22	a	2573	C
22	a	2582	G
22	a	2585	U
22	a	2586	U
22	a	2602	A
22	a	2603	G
22	a	2609	U
22	a	2613	U
22	a	2615	U
22	a	2629	U
22	a	2630	G

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Mol	Chain	Res	Type
22	a	2639	A
22	a	2646	C
22	a	2661	G
22	a	2689	U
22	a	2690	U
22	a	2713	U
22	a	2714	G
22	a	2726	A
22	a	2732	G
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2758	A
22	a	2765	A
22	a	2778	A
22	a	2791	G
22	a	2797	U
22	a	2798	U
22	a	2799	A
22	a	2820	A
22	a	2835	A
22	a	2849	U
22	a	2861	U
22	a	2873	A
22	a	2880	C
22	a	2883	A
22	a	2884	U
22	a	2901	C
23	b	9	G
23	b	34	A
23	b	35	C
23	b	37	C
23	b	41	G
23	b	56	G
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	108	A
23	b	109	A
54	X	19	U
55	Y	10	G

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Mol	Chain	Res	Type
55	Y	14	A
55	Y	46	G
55	Y	48	C
55	Y	49	G
55	Y	52	G
55	Y	58	A
55	Y	66	C
55	Y	68	G
55	Y	70	U
55	Y	71	C
55	Y	76	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	264	C

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

41 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	$\# Z > 2$
1	5MC	A	1407	1	18,22,23	0.31	0	26,32,35	0.45	0
1	MA6	A	1518	1	23,26,27	0.33	0	34,38,41	0.63	1 (2%)
1	2MG	A	1207	1	23,26,27	0.28	0	32,38,41	0.35	0
22	H2U	a	2449	22	18,21,22	0.46	0	21,30,33	1.03	1 (4%)
22	OMG	a	2251	58,55,22	23,26,27	0.29	0	33,38,41	0.37	0
1	PSU	A	516	1	18,21,22	0.50	0	22,30,33	0.61	1 (4%)
22	2MG	a	1835	22	23,26,27	0.28	0	32,38,41	0.33	0
33	MS6	l	82	33	5,7,8	0.31	0	2,7,9	0.06	0
22	OMC	a	2498	22,57	19,22,23	0.32	0	26,31,34	0.39	0
53	FME	W	1	53	8,9,10	0.50	0	7,9,11	0.47	0
22	5MC	a	1962	58,22	18,22,23	0.30	0	26,32,35	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	4D4	l	81	33	9,11,12	0.84	0	8,13,15	1.93	3 (37%)
22	PSU	a	2604	22	18,21,22	0.54	0	22,30,33	0.58	0
12	D2T	L	89	12	7,9,10	0.88	0	6,11,13	1.70	2 (33%)
22	5MU	a	747	22	19,22,23	0.28	0	28,32,35	0.33	0
22	6MZ	a	2030	22	22,25,26	0.27	0	30,36,39	0.43	0
22	PSU	a	2605	22	18,21,22	0.52	0	22,30,33	0.62	0
22	PSU	a	1911	22	18,21,22	0.47	0	22,30,33	0.58	0
22	5MU	a	1939	58,22	19,22,23	0.28	0	28,32,35	0.38	0
22	3TD	a	1915	22	18,22,23	0.47	0	22,32,35	0.59	0
22	PSU	a	746	22,57	18,21,22	0.58	1 (5%)	22,30,33	0.67	1 (4%)
22	6MZ	a	1618	22	22,25,26	0.26	0	30,36,39	0.44	0
22	G7M	a	2069	58,22	23,26,27	0.34	0	35,39,42	0.48	0
25	MEQ	d	150	25	8,9,10	0.87	0	5,10,12	0.46	0
22	2MA	a	2503	22,57	22,25,26	0.97	1 (4%)	33,37,40	1.33	3 (9%)
1	4OC	A	1402	1	20,23,24	0.32	0	26,32,35	0.46	0
11	IAS	K	119	11	6,7,8	0.74	0	6,8,10	0.96	0
22	PSU	a	2580	22	18,21,22	0.58	1 (5%)	22,30,33	0.67	1 (4%)
1	MA6	A	1519	1	23,26,27	0.30	0	34,38,41	0.63	1 (2%)
1	2MG	A	1516	1	23,26,27	0.28	0	32,38,41	0.39	0
22	PSU	a	1917	22	18,21,22	0.50	0	22,30,33	0.56	0
22	PSU	a	2504	22	18,21,22	0.49	0	22,30,33	0.59	0
22	OMU	a	2552	22	19,22,23	0.28	0	26,31,34	0.43	0
22	PSU	a	2457	22	18,21,22	0.50	0	22,30,33	0.60	1 (4%)
1	2MG	A	966	1	23,26,27	0.29	0	32,38,41	0.37	0
1	UR3	A	1498	1	19,22,23	0.30	0	26,32,35	0.37	0
22	PSU	a	955	58,22	18,21,22	0.48	0	22,30,33	0.58	0
22	1MG	a	745	22	22,26,27	0.29	0	33,39,42	0.60	1 (3%)
22	2MG	a	2445	22	23,26,27	0.31	0	32,38,41	0.33	0
1	5MC	A	967	1	18,22,23	0.29	0	26,32,35	0.44	0
1	G7M	A	527	1	23,26,27	0.33	0	35,39,42	0.48	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
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	1/11/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
22	H2U	a	2449	22	-	1/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMG	a	2251	58,55,22	-	1/9/27/28	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
33	MS6	l	82	33	-	1/4/6/8	-
22	OMC	a	2498	22,57	-	0/9/27/28	0/2/2/2
53	FME	W	1	53	-	3/7/9/11	-
22	5MC	a	1962	58,22	-	0/7/25/26	0/2/2/2
33	4D4	l	81	33	-	5/11/12/14	-
22	PSU	a	2604	22	-	2/7/25/26	0/2/2/2
12	D2T	L	89	12	-	2/7/12/14	-
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	5MU	a	1939	58,22	-	0/7/25/26	0/2/2/2
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
22	PSU	a	746	22,57	-	2/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
22	G7M	a	2069	58,22	-	1/7/25/26	0/3/3/3
25	MEQ	d	150	25	-	5/8/9/11	-
22	2MA	a	2503	22,57	-	1/7/25/26	0/3/3/3
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
11	IAS	K	119	11	-	2/7/7/8	-
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	3/11/29/30	0/3/3/3
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2504	22	-	2/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	0/9/27/28	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
22	PSU	a	955	58,22	-	0/7/25/26	0/2/2/2
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
22	2MG	a	2445	22	-	0/9/27/28	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	1/7/25/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2503	2MA	C6-N6	-3.24	1.26	1.34
22	a	746	PSU	O4'-C1'	-2.16	1.40	1.43
22	a	2580	PSU	O4'-C1'	-2.06	1.41	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2503	2MA	N6-C6-N1	4.60	123.53	117.03
33	l	81	4D4	NE-CZ-NH2	3.90	127.56	120.70
22	a	2503	2MA	C2-N1-C6	3.80	124.00	118.08
22	a	2503	2MA	C5-C6-N1	-3.52	112.94	119.01
22	a	2449	H2U	C5-C4-N3	-3.12	113.15	116.65
12	L	89	D2T	O-C-CA	-2.76	117.56	124.78
33	l	81	4D4	NH1-CZ-NE	-2.67	113.02	119.19
33	l	81	4D4	O-C-CA	-2.66	117.80	124.78
22	a	745	1MG	C6-C5-C4	-2.63	117.06	119.97
1	A	1519	MA6	C2-N1-C6	2.42	117.46	111.75
12	L	89	D2T	OD1-CG-CB	-2.41	117.39	122.44
1	A	1518	MA6	C2-N1-C6	2.36	117.33	111.75
22	a	2580	PSU	O4'-C1'-C2'	2.31	108.40	105.14
22	a	746	PSU	O4'-C1'-C2'	2.26	108.33	105.14
1	A	516	PSU	O4'-C1'-C2'	2.10	108.11	105.14
22	a	2457	PSU	O4'-C1'-C2'	2.06	108.05	105.14

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	C5-C6-N6-C10
12	L	89	D2T	CG-CB-SB-CB1
33	l	81	4D4	N-CA-CB-CG
33	l	81	4D4	NH2-CZ-NE-CD
22	a	2251	OMG	C1'-C2'-O2'-CM2
22	a	2504	PSU	O4'-C4'-C5'-O5'
53	W	1	FME	O1-CN-N-CA
53	W	1	FME	C-CA-CB-CG
22	a	2030	6MZ	O4'-C4'-C5'-O5'
22	a	2504	PSU	C3'-C4'-C5'-O5'
25	d	150	MEQ	CA-CB-CG-CD
22	a	2030	6MZ	C3'-C4'-C5'-O5'
22	a	2604	PSU	C3'-C4'-C5'-O5'
33	l	82	MS6	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	C5-C6-N6-C10
1	A	1519	MA6	C5-C6-N6-C9
53	W	1	FME	N-CA-CB-CG
22	a	2604	PSU	O4'-C4'-C5'-O5'
25	d	150	MEQ	OE1-CD-CG-CB
25	d	150	MEQ	N-CA-CB-CG
33	l	81	4D4	NH1-CZ-NE-CD
11	K	119	IAS	OXT-C-CA-CB
11	K	119	IAS	O-C-CA-CB
25	d	150	MEQ	NE2-CD-CG-CB
1	A	1519	MA6	O4'-C4'-C5'-O5'
22	a	2503	2MA	O4'-C4'-C5'-O5'
22	a	746	PSU	O4'-C1'-C5-C4
22	a	2069	G7M	O4'-C4'-C5'-O5'
12	L	89	D2T	CA-CB-SB-CB1
22	a	2449	H2U	C4'-C5'-O5'-P
25	d	150	MEQ	C-CA-CB-CG
33	l	81	4D4	C-CA-CB-OB
22	a	746	PSU	O4'-C4'-C5'-O5'
33	l	81	4D4	C-CA-CB-CG
1	A	527	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	2251	OMG	1	0
1	A	516	PSU	1	0
12	L	89	D2T	3	0
22	a	2030	6MZ	2	0
22	a	2503	2MA	1	0
1	A	1402	4OC	1	0
1	A	966	2MG	1	0
22	a	745	1MG	1	0
1	A	967	5MC	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 357 ligands modelled in this entry, 349 are monoatomic - leaving 8 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	SPD	a	6199	-	9,9,9	0.19	0	8,8,8	0.78	0
59	SPD	a	6195	-	9,9,9	0.27	0	8,8,8	0.85	0
59	SPD	a	6194	-	9,9,9	0.25	0	8,8,8	0.88	0
59	SPD	a	6197	-	9,9,9	0.22	0	8,8,8	0.89	0
59	SPD	a	6198	-	9,9,9	0.23	0	8,8,8	0.87	0
59	SPD	a	6196	-	9,9,9	0.29	0	8,8,8	0.82	0
60	PUT	a	6200	-	5,5,5	0.12	0	4,4,4	0.16	0
59	SPD	a	6193	-	9,9,9	0.30	0	8,8,8	0.89	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	SPD	a	6199	-	-	0/7/7/7	-
59	SPD	a	6195	-	-	0/7/7/7	-
59	SPD	a	6194	-	-	0/7/7/7	-
59	SPD	a	6197	-	-	3/7/7/7	-
59	SPD	a	6198	-	-	0/7/7/7	-
59	SPD	a	6196	-	-	1/7/7/7	-
60	PUT	a	6200	-	-	0/3/3/3	-
59	SPD	a	6193	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	a	6197	SPD	C3-C4-C5-N6
59	a	6197	SPD	N6-C7-C8-C9
59	a	6197	SPD	C4-C5-N6-C7
59	a	6196	SPD	N6-C7-C8-C9

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	a	6199	SPD	1	0
59	a	6197	SPD	3	0
59	a	6196	SPD	2	0
59	a	6193	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.

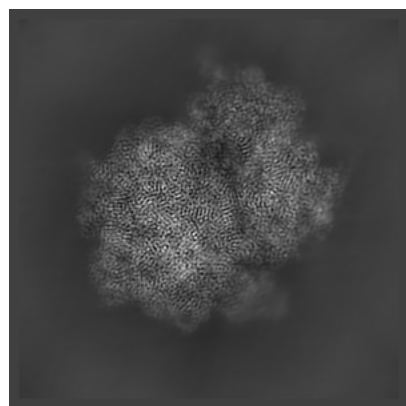
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60473. These allow visual inspection of the internal detail of the map and identification of artifacts.

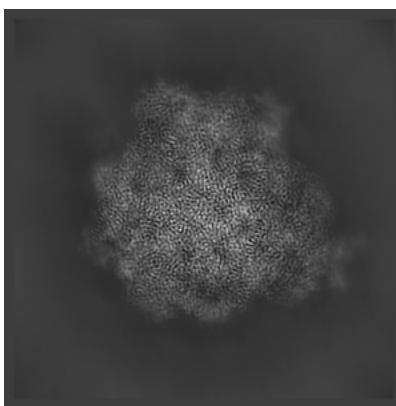
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

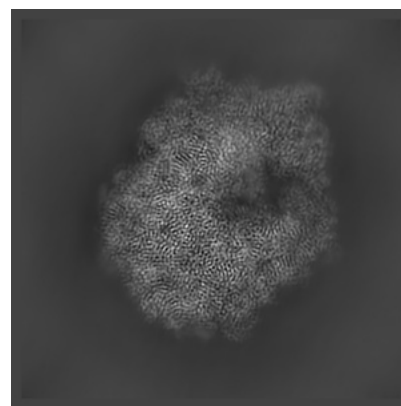
6.1.1 Primary map



X

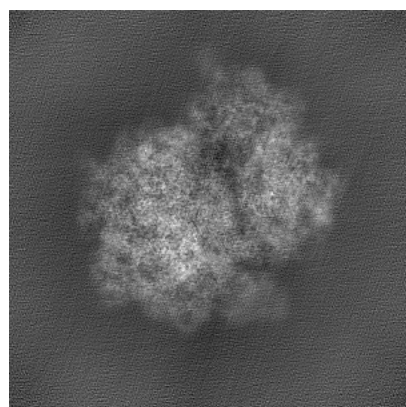


Y

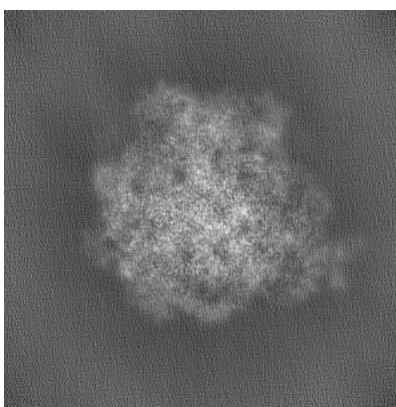


Z

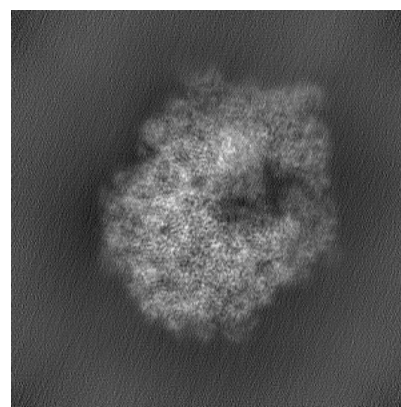
6.1.2 Raw map



X



Y

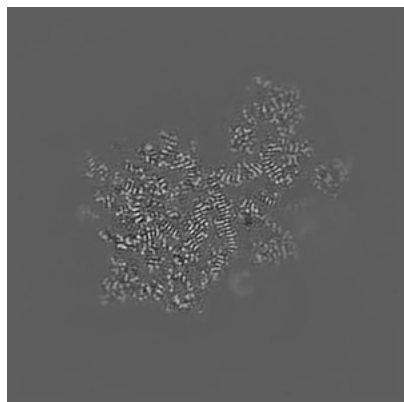


Z

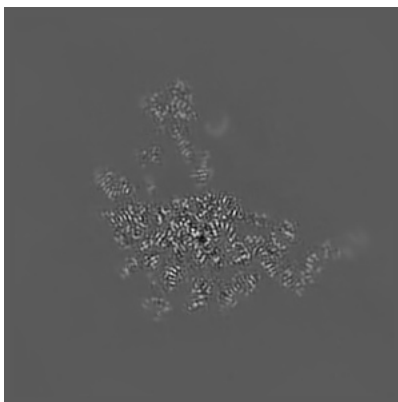
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

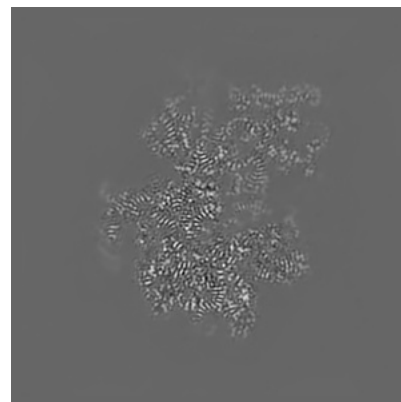
6.2.1 Primary map



X Index: 216

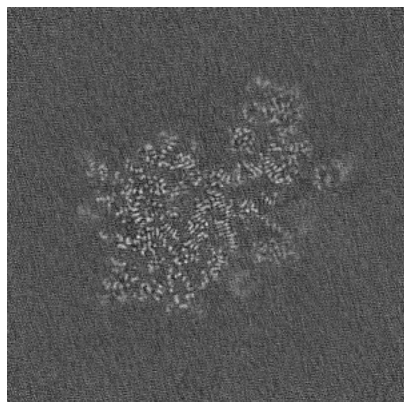


Y Index: 216

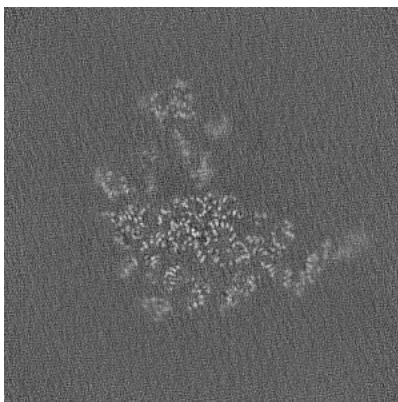


Z Index: 216

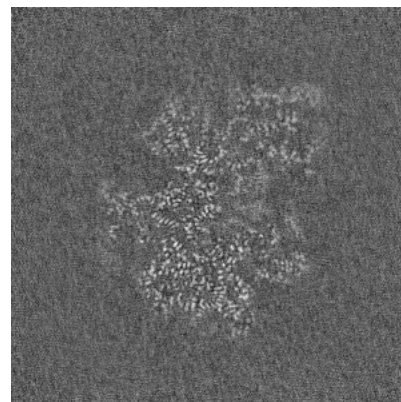
6.2.2 Raw map



X Index: 216



Y Index: 216

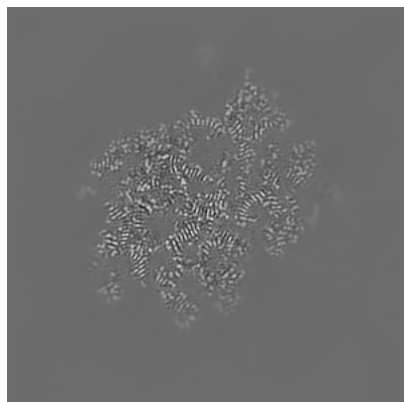


Z Index: 216

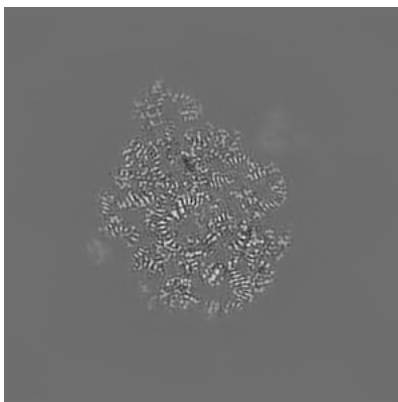
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

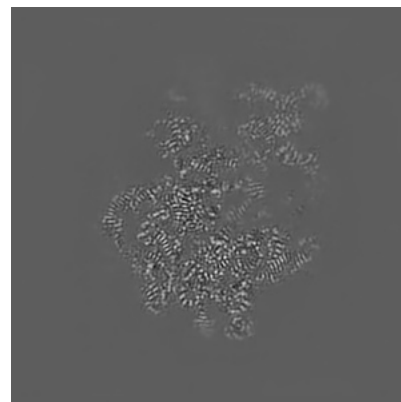
6.3.1 Primary map



X Index: 186

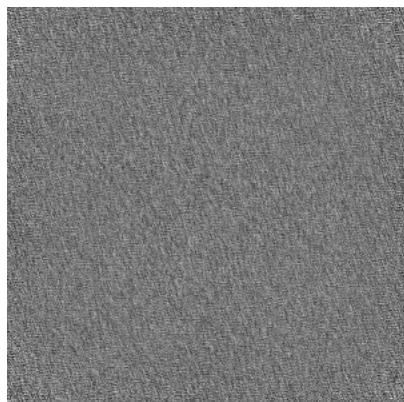


Y Index: 178

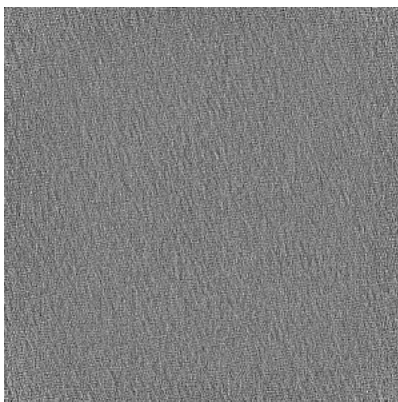


Z Index: 208

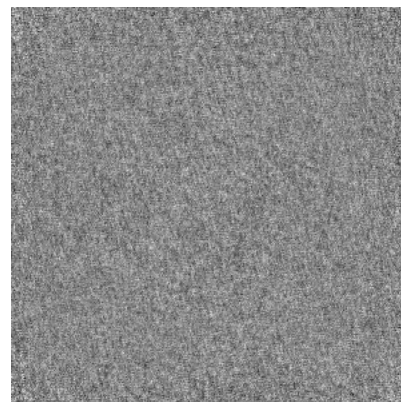
6.3.2 Raw map



X Index: 0



Y Index: 0

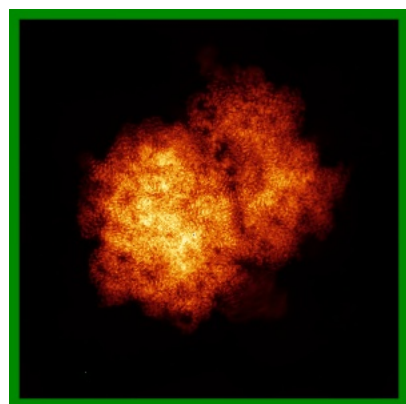


Z Index: 0

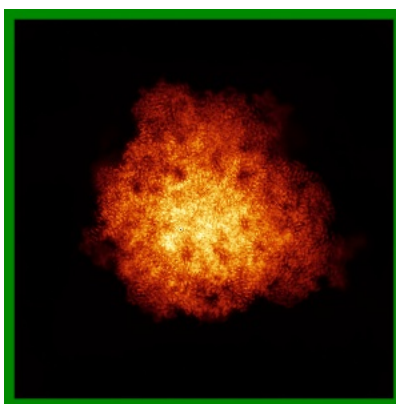
The images above show the largest variance slices of the map in three orthogonal directions.

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

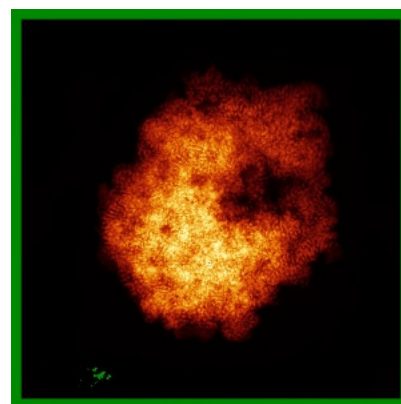
6.4.1 Primary map



X

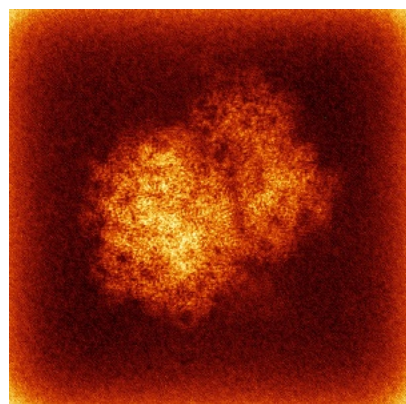


Y

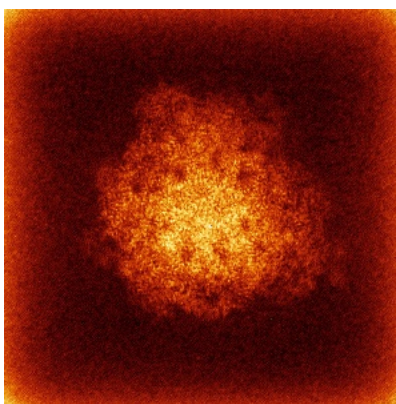


Z

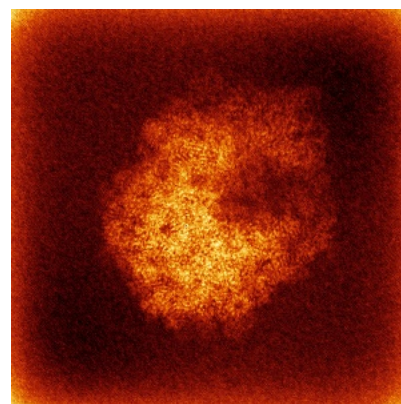
6.4.2 Raw map



X



Y

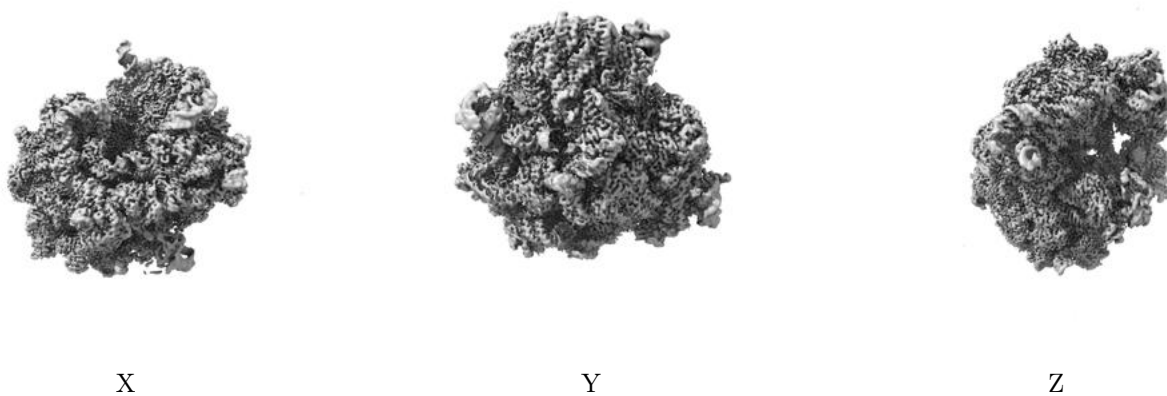


Z

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

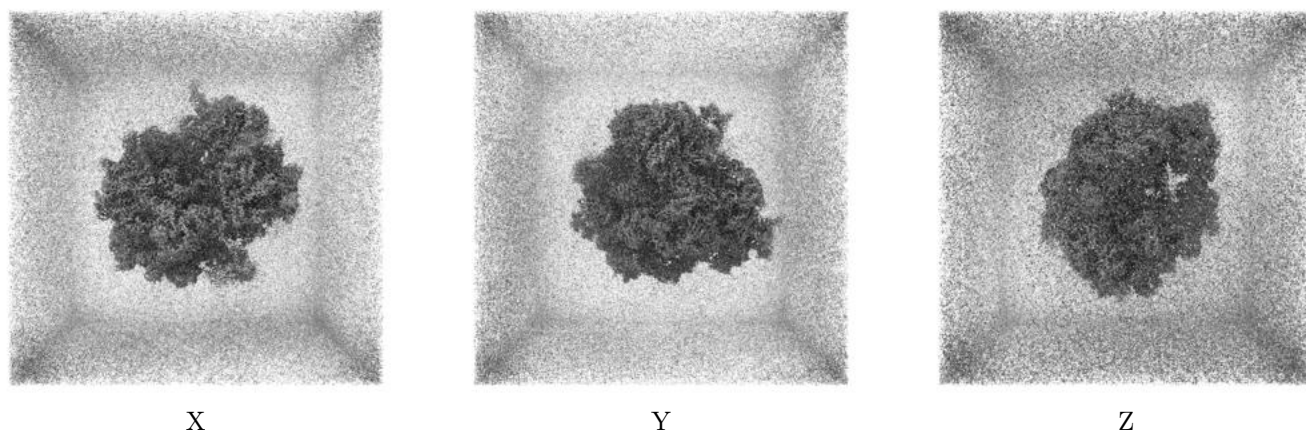
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

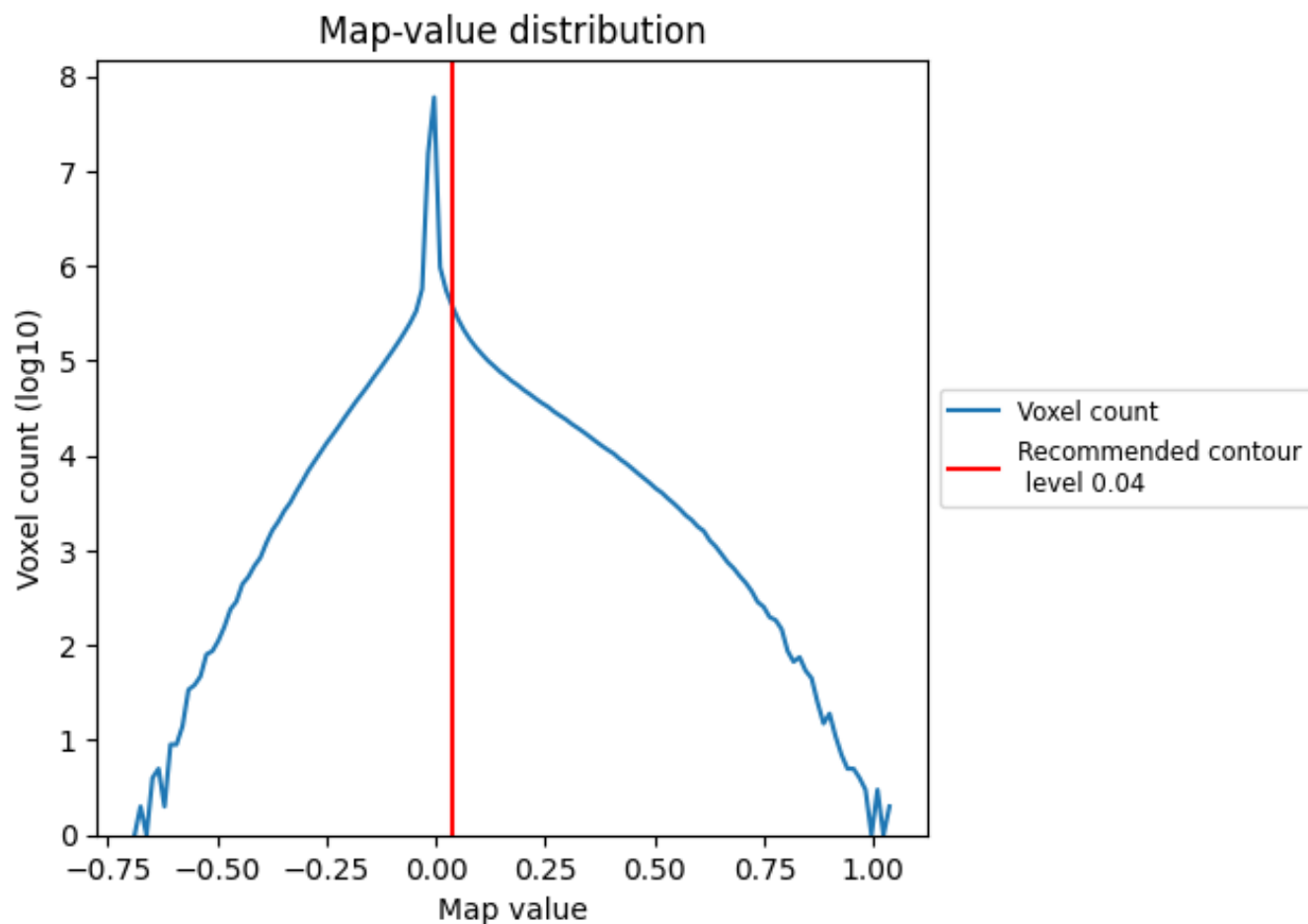
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

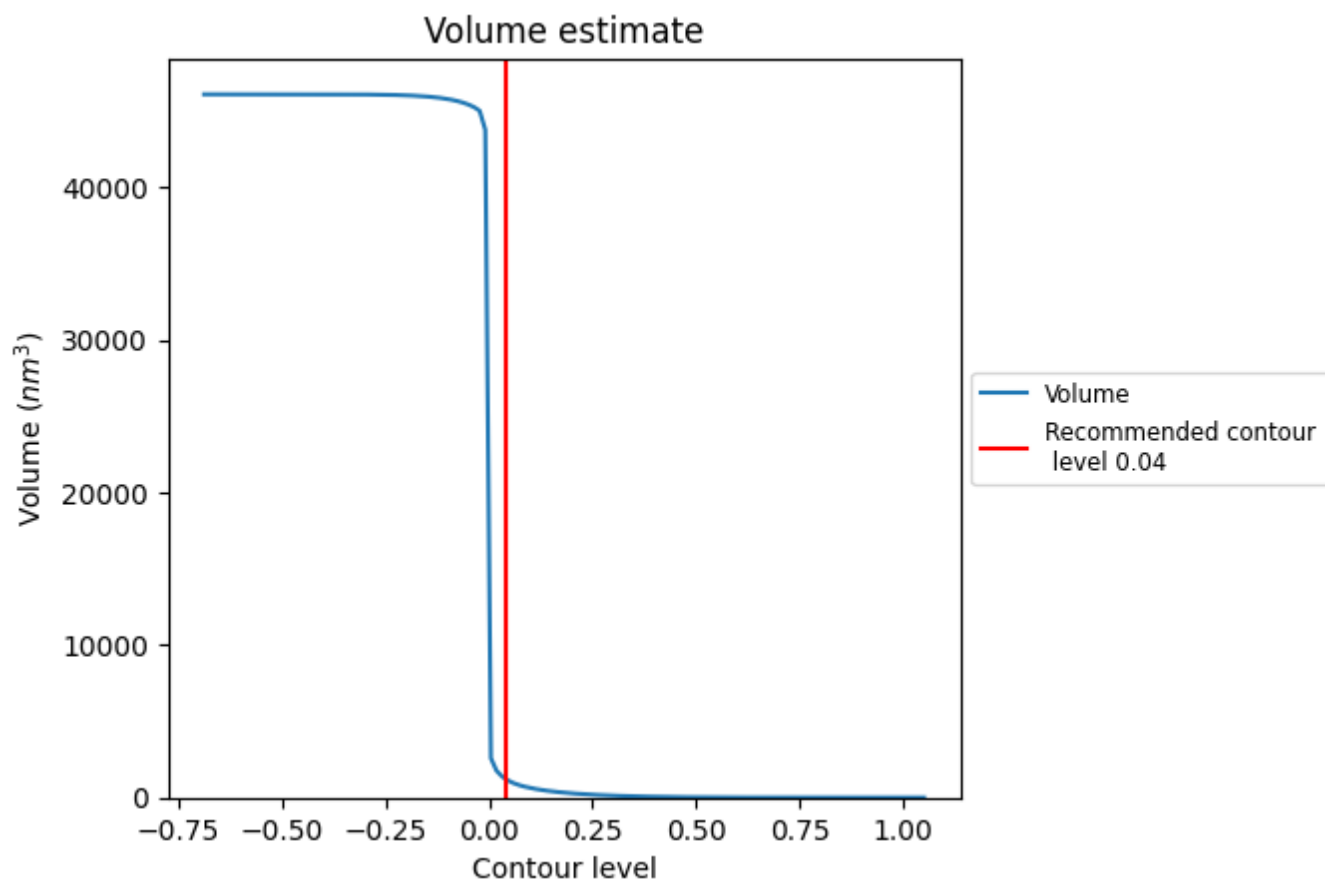
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

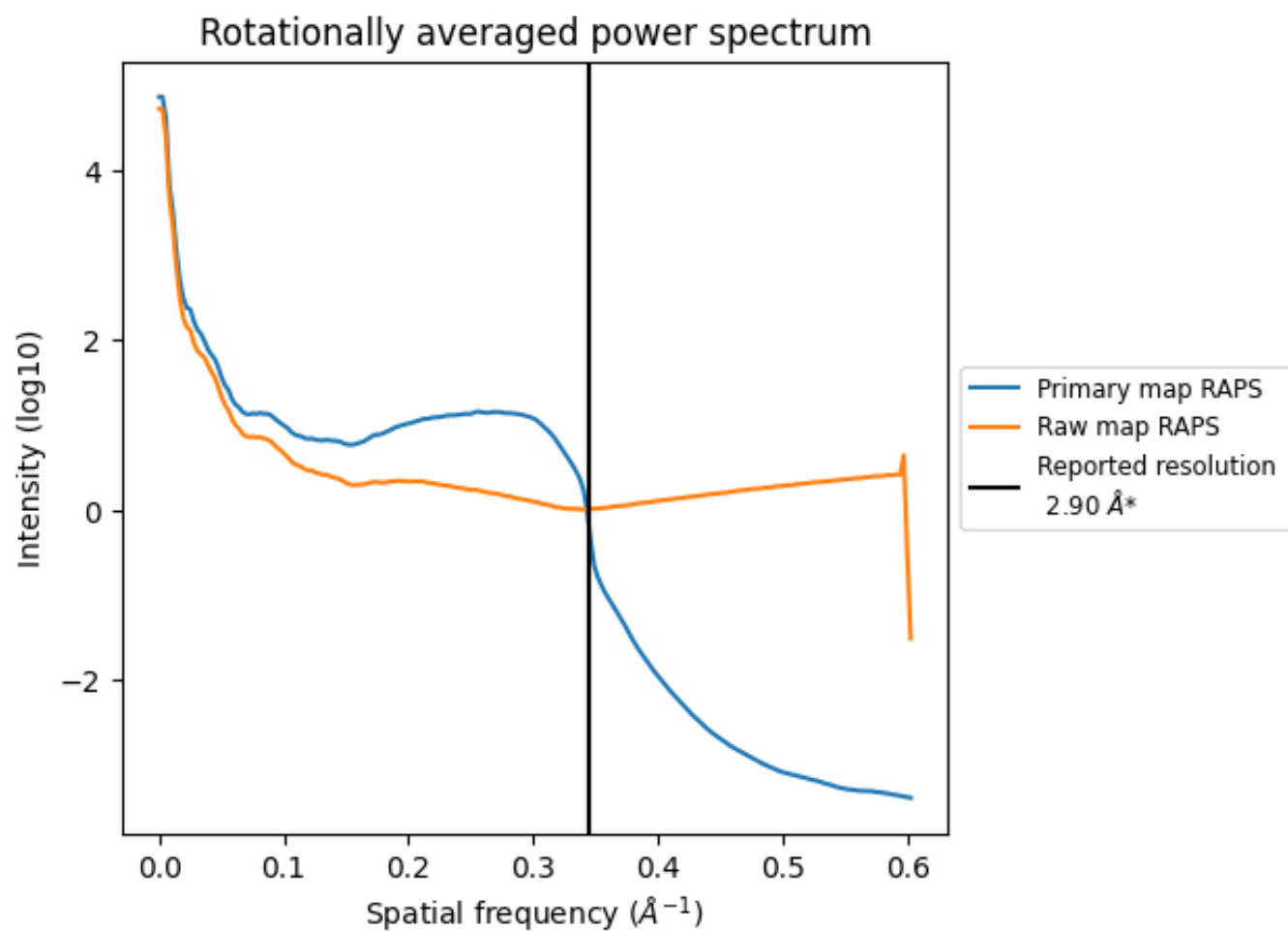
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1224 nm³; this corresponds to an approximate mass of 1106 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 ⓘ

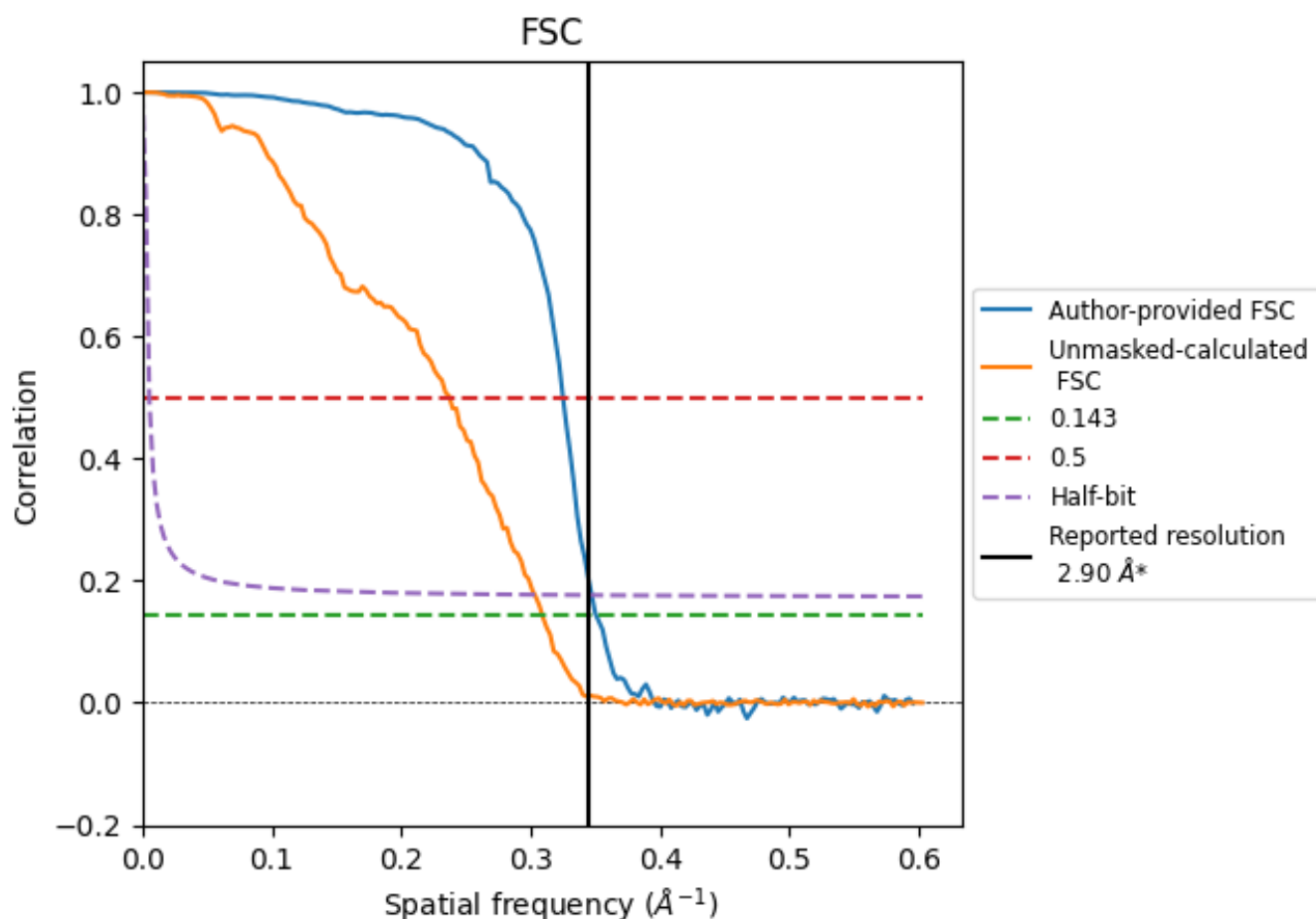


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

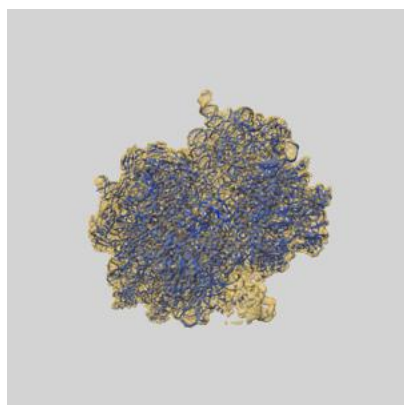
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.85	3.08	2.88
Unmasked-calculated*	3.24	4.21	3.30

*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 3.24 differs from the reported value 2.9 by more than 10 %

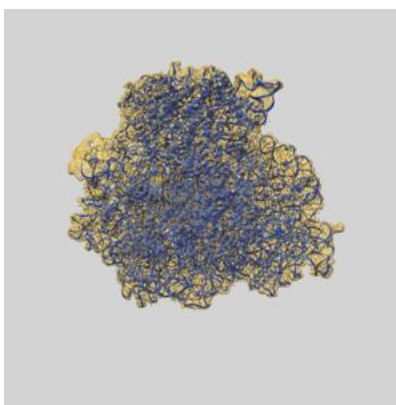
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60473 and PDB model 8ZTU. Per-residue inclusion information can be found in section [3](#) on page [17](#).

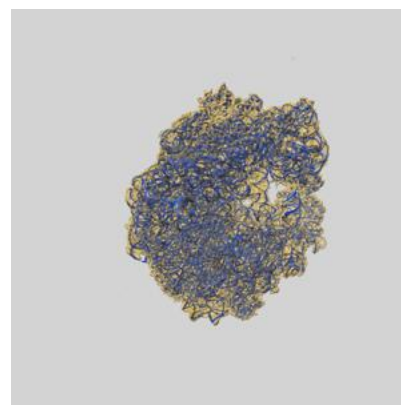
9.1 Map-model overlay [i](#)



X



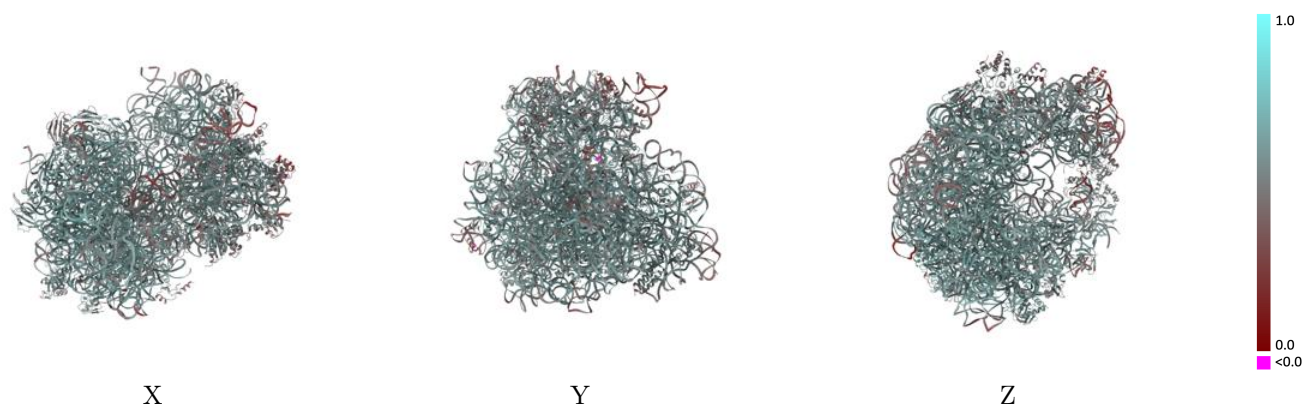
Y



Z

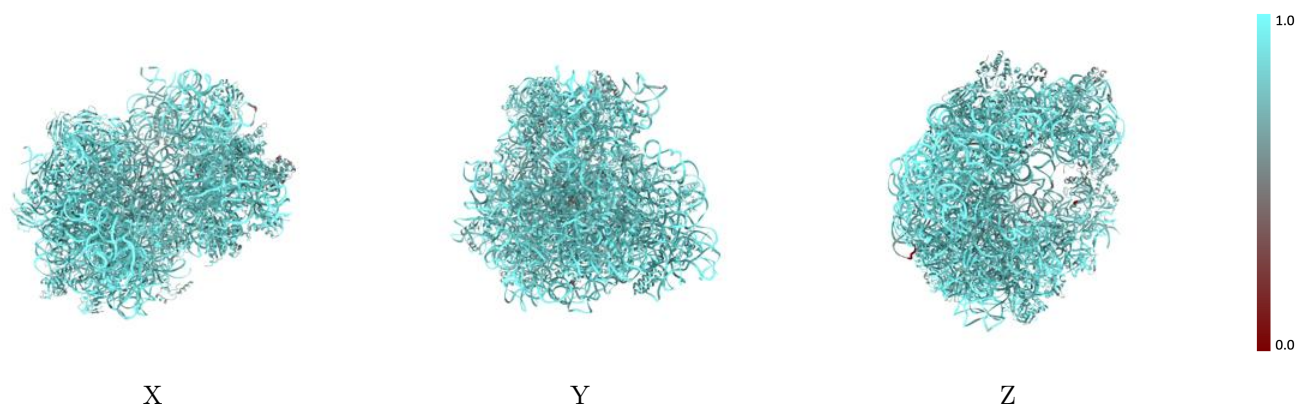
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



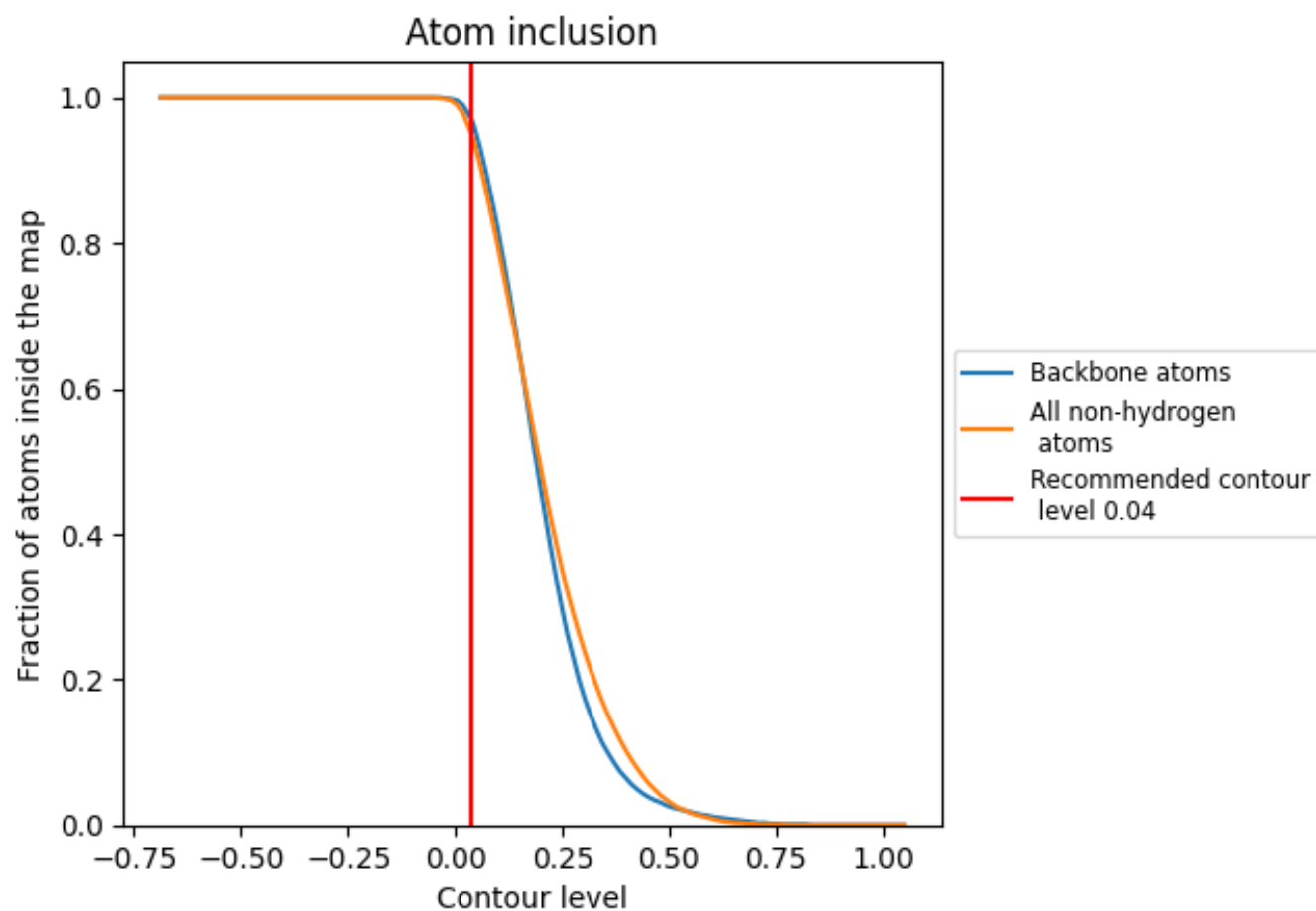
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9480	 0.5710
0	 0.9050	 0.5580
1	 0.9660	 0.6250
2	 0.9550	 0.6130
3	 0.9420	 0.5840
4	 0.8070	 0.4660
A	 0.9680	 0.5620
B	 0.7970	 0.4690
C	 0.8800	 0.5300
D	 0.8640	 0.5160
E	 0.9110	 0.5640
F	 0.8470	 0.5120
G	 0.8400	 0.4850
H	 0.8900	 0.5490
I	 0.8530	 0.4880
J	 0.7620	 0.4360
K	 0.9030	 0.5510
L	 0.9100	 0.5560
M	 0.8240	 0.4940
N	 0.8610	 0.5060
O	 0.9010	 0.5510
P	 0.8950	 0.5440
Q	 0.8800	 0.5310
R	 0.8740	 0.5400
S	 0.8220	 0.5010
T	 0.8840	 0.5260
U	 0.7480	 0.4570
W	 0.8780	 0.5120
X	 0.7270	 0.4410
Y	 0.8870	 0.5050
Z	 0.9290	 0.5800
a	 0.9790	 0.5980
b	 0.9710	 0.5680
c	 0.9620	 0.6060
d	 0.9490	 0.5930



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Chain	Atom inclusion	Q-score
e	 0.8930	 0.5560
f	 0.8380	 0.4970
g	 0.8440	 0.4930
h	 0.7490	 0.4250
i	 0.9530	 0.6000
j	 0.9470	 0.5900
k	 0.9380	 0.5870
l	 0.9500	 0.5920
m	 0.9710	 0.6140
n	 0.9030	 0.5410
o	 0.9350	 0.5890
p	 0.9660	 0.6130
q	 0.9280	 0.5810
r	 0.9330	 0.5850
s	 0.9040	 0.5660
t	 0.8940	 0.5430
u	 0.8770	 0.5350
v	 0.9240	 0.5840
w	 0.9430	 0.5910
x	 0.8730	 0.5330
y	 0.9130	 0.5880
z	 0.9440	 0.5970